COSMO*logic* GmbH & Co. KG

Computational Chemistry and Fluid Thermodynamics

TmoleX

A Graphical User Interface to the

TURBOMOLE

Quantum Chemistry Program Package

User manual

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1. Installation

1.1. Windows

Prerequisites: Windows XP, Windows Vista, Windows 7 or Windows HPC2008

The Windows version of TmoleX is distributed as a single executable file, called TmoleX_windows_3_0.exe. To install TmoleX, simply double-click on TmoleX_windows_3_0.exe and follow the installation instructions.

After installation, TmoleX is available in your Windows Start Menu or as an icon on your desktop.

Please Note :

TURBOMOLE 6.2 for Windows is included in the TmoleX package. You will not have to install it additionally. Some features of TURBOMOLE that are based on classical Unix scripts are not yet ported to Windows:

- Numerical second derivatives (script NumForce)
- automatic BSSE calculations (program jobbsse)

The TURBOMOLE version for Windows(32bit) includes one generic type of serial 32-bit executable only, without special optimization for a certain type of CPU. It runs on any processor that is compatible to the Pentium 4 instruction set which supports SSE2.

The TURBOMOLE version for Windows(64bit) includes serial and parallel 64-bit executables. The parallel MPI version is only functional on Windows HPC systems with an installed version MS-MPI.

1.2. Linux

Prerequisites: Linux distribution based on Kernel 2.6.x

The Linux version of TmoleX is distributed as a single file called TmoleX_linux_3_0.sh. Please make sure that the file has execute permissions (chmod a+rx TmoleX_linux_3_0.sh) before starting it, then follow the instructions on screen.

The full version of TURBOMOLE 6.2 is included in the TmoleX package. Optimized binaries for a 32-bit (Pentium compatible CPUs) and 64-bit platforms (AMD64 and EM64T) are available and will be chosen automatically by the script sysname.

Features that are not supported by TmoleX can be used by the command line version. After the installation of TmoleX, TURBOMOLE can be used from the command line as usual. Just set `$TURBODIR` to the TURBOMOLE directory of the TmoleX installation, and extend the PATH to `$TURBODIR/scripts` and `$TURBODIR/bin/`sysname`` (the binary directory).

1.3. Mac OS

Prerequisites: Mac OS X 10.5.

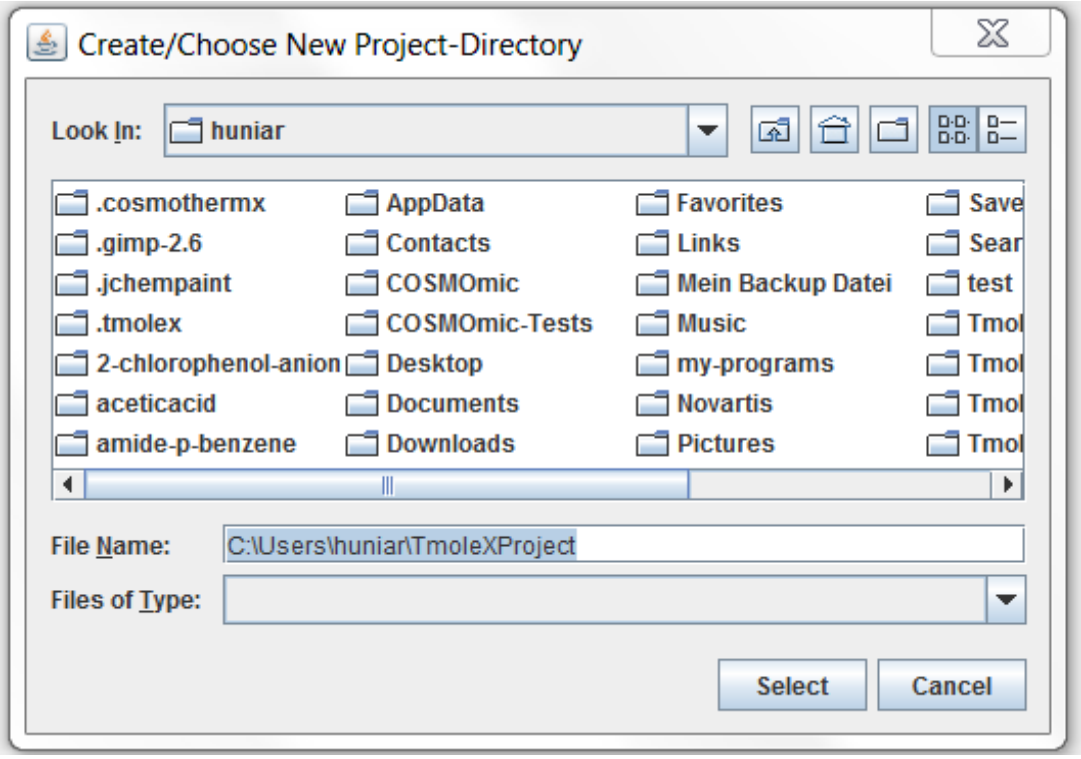
The Mac OS version of TmoleX is distributed as a single file called TmoleX_macos_3_0.dmg. To install TmoleX, simply double-click on TmoleX_macos_3_0 and follow the installation instructions.

After installation, TmoleX is available in the chosen folder (by default in /Application/COSMOlogic/TmoleX3). Features that are not supported by TmoleX can be used by the command line version. After the installation of TmoleX, TURBOMOLE can be used from the command line as usual. Just set `$TURBODIR` to the TURBOMOLE directory of the TmoleX installation, and extend the PATH to `$TURBODIR/scripts` and `$TURBODIR/bin/`sysname`` (the binary directory).

2. A quick tour

2.1. Starting the program

Starting TmoleX for the first time, you will be asked to choose a directory for your first project.



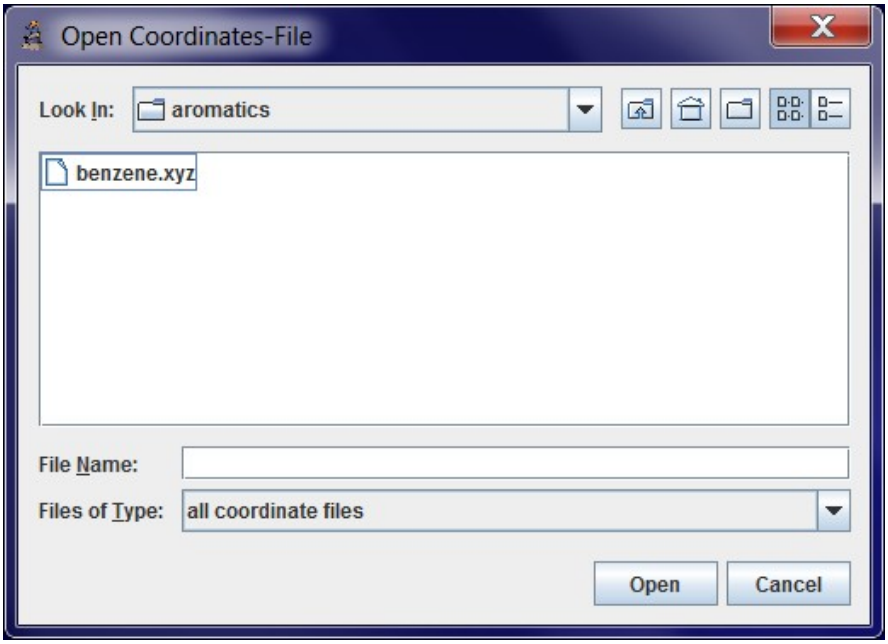
The default directory is called TmoleXProject in your home folder. Just click on Select to accept the default or generate a new directory and choose this one.

2.2. An illustrative example: Part 1

This section will guide you through the process of performing a DFT energy calculation and a ground state geometry optimization of a molecule, for which input coordinates exist, e.g. benzene.

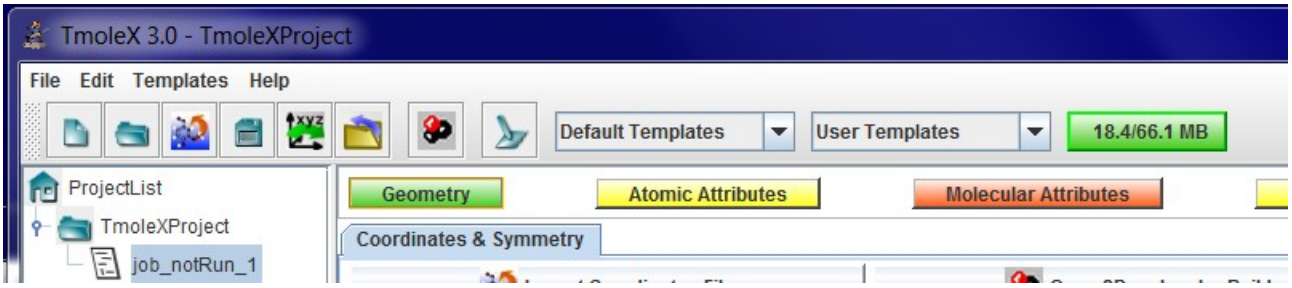
The button

in the tool bar or the menu 'Import Coordinate File' in the pull-down menu 'File' will open a file browser.



Select the coordinate file and load the molecular structure of benzene in TmoleX (first change to the installation directory COSMOlogic10/TmoleX/prefabs/aromatics).

2.3. The tool bar



The tools in the tool bar act only on the job that you are currently working on, i.e. which is opened in the project list.

Create new job within the current project.

Open existing control file – either from an existing job directory or from external sources.

Read or import coordinates (besides TURBOMOLE also xyz, car, sdf, ml2, arc, cosmo, chem3d format).

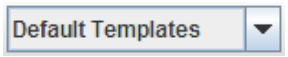
Save current job to disk (file browser is being opened).

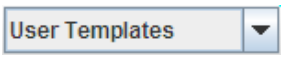
Save/Export current coordinates in various formats.

Open the directory of the current job in the default file browser of your OS.

Open molecular viewer. Can also be used to build new molecules.

Edit control file – this is the central input file for TURBOMOLE jobs .This feature can be used to change or add keywords, i.e. also to add features that are not directly supported by TmoleX.





Job templates. Choosing a template from the default ones that come with TmoleX or from the ones the user has saved before, will automatically set up a job with saved default settings. See chapter 6 for details about templates.

2.4. The sections

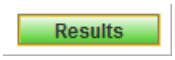
TmoleX is structured as an interactive TURBOMOLE input program, similar to the 'define' program, which generates the input on the command line.

1. On the left you will find a list of open projects and jobs of each project,
2. on the top the general task menu (Geometry, Atomic Attributes, Molecular Attributes, etc.)
3. in the main frame the data assigned to the chosen task.

The input is divided into four different sections:

The kind of job or property that shall be calculated can be set in the Start Job panel:

Results after a successful run can be viewed and further investigated in the Results panel:



You should follow the menu structure in the main frame from left to right. The traffic light colours are indicating which steps have been accomplished and for which steps input is needed.

Color code

Red: No valid data is available. User action required.

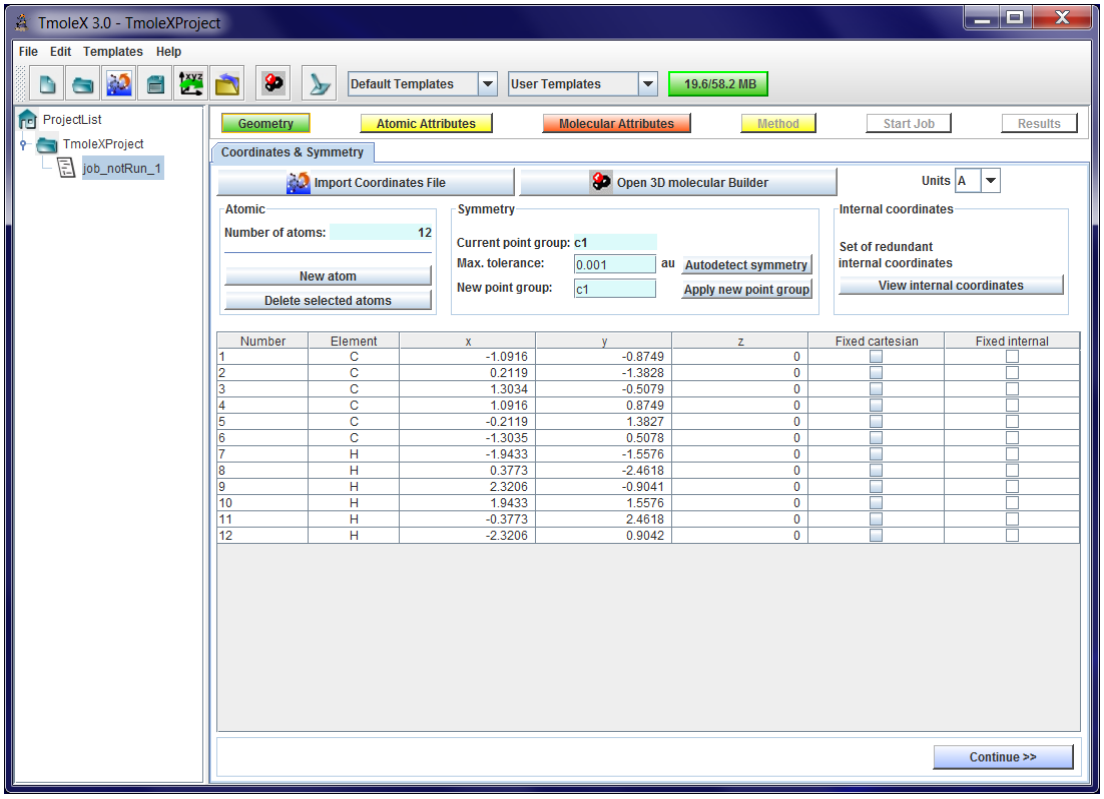
Yellow: Default settings available – unchecked by user so far.

Green: The data is correct or user did already visit this section.

2.5. An illustrative example: Part 2

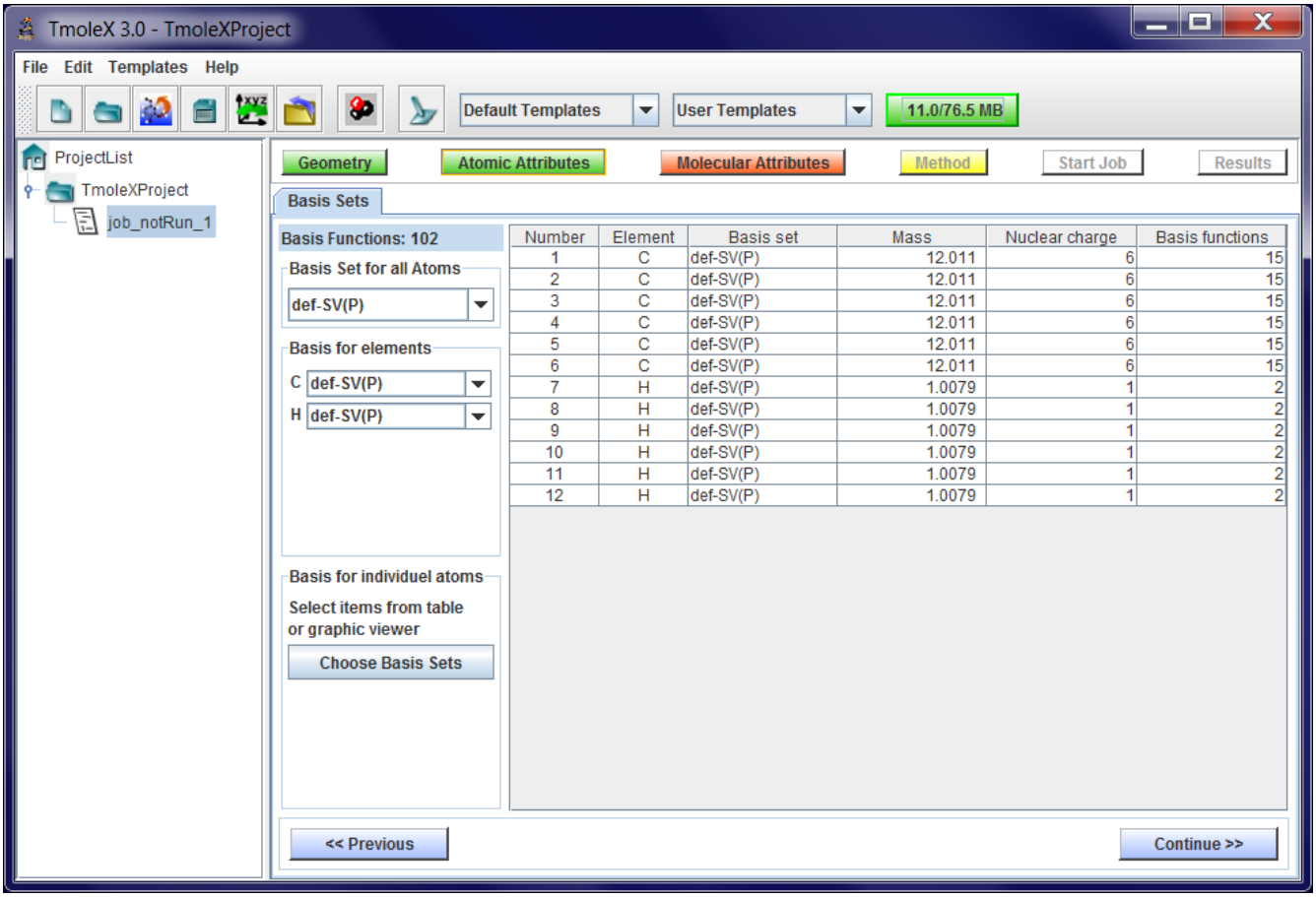
2.5.1 Geometry panel

After reading in the coordinates, you are in the Geometry section. Here, you can choose the symmetry, create internal coordinates, add atoms, or modify the structure.



2.5.2 Basis set panel

The basis set is being defined in the Atomic Attributes panel:



The basis set is def-SV(P) by default for all atoms. You have the possibility to select one basis for all atoms, basis sets for given elements, or basis sets for individual marked atoms.

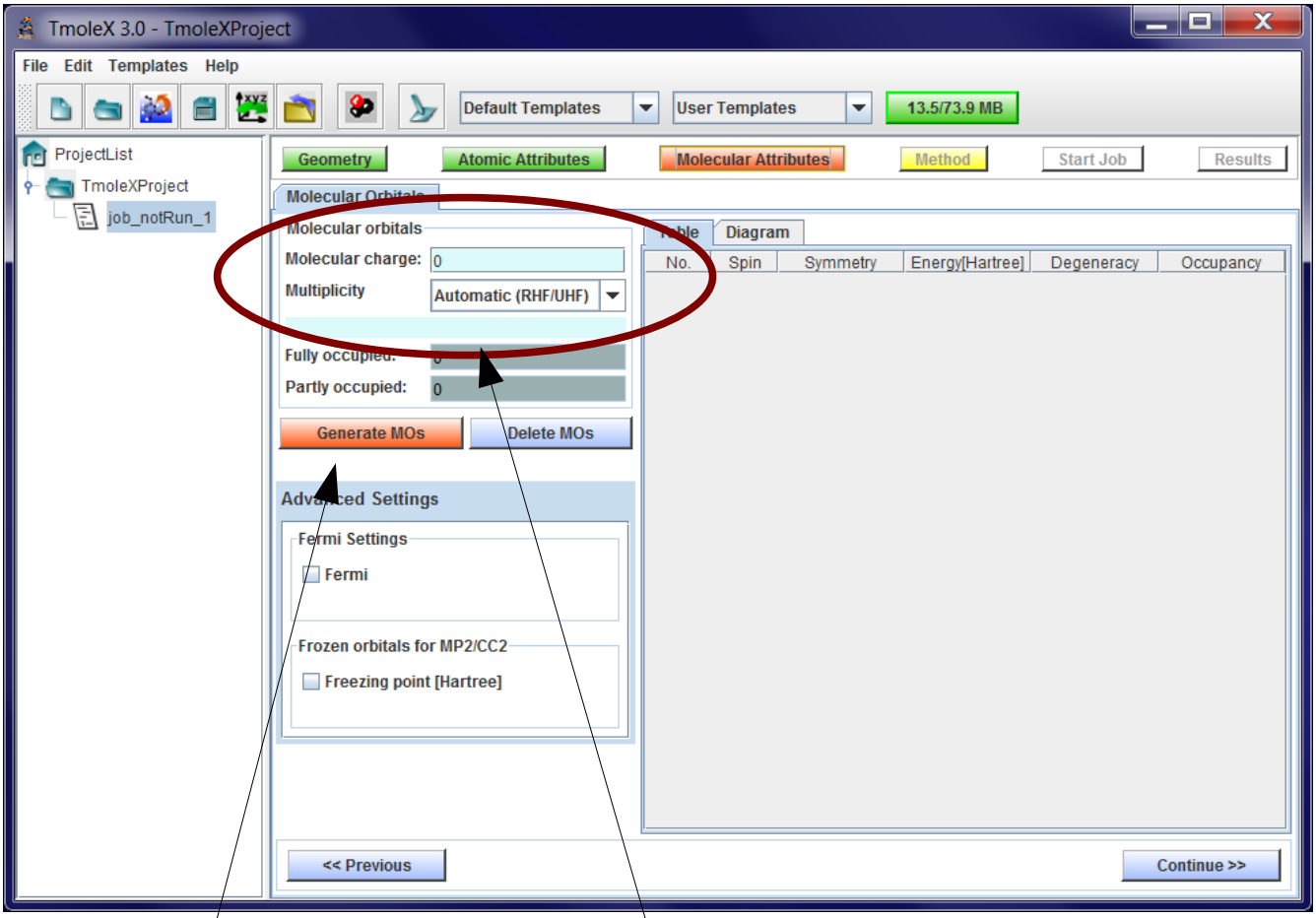
Hint:

If you are not familiar with the modern Ahlrichs type basis sets but with old Pople type basis sets only:

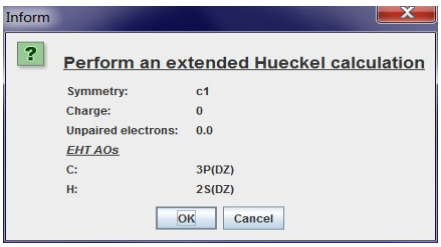
6-31G*	is of similar quality than	def-SV(P),
6-31G**	--	def-SVP, and
6-311G**	--	def-TZVP.

2.5.3 Molecular start orbitals panel

For any TURBOMOLE calculation an initial set of molecular orbitals is required. This is done with an extended Hückel calculation in the Molecular Attributes panel. If you do not (yet) have valid start orbitals, the button will remain red.

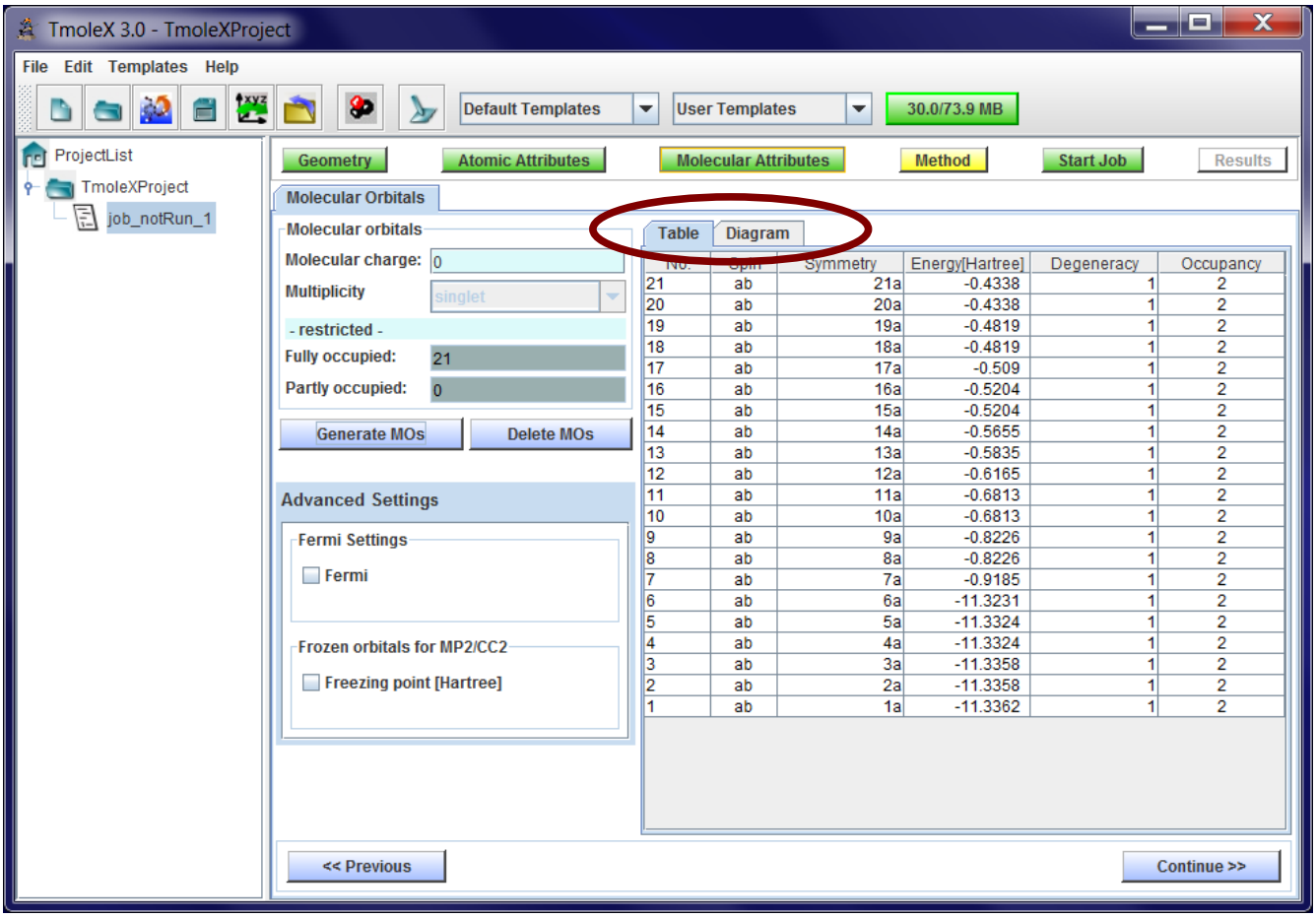


If you click on 'Generate MOs', a message box will come up



Do not forget to set the molecular total charge before generating orbitals for IONS !!

Click 'Ok'. The generation takes only a (very) short time to compute and the initial molecular orbital are displayed.



No.	Spin	Symmetry	Energy[Hartree]	Degeneracy	Occupancy
21	ab	21a	-0.4338	1	2
20	ab	20a	-0.4338	1	2
19	ab	19a	-0.4819	1	2
18	ab	18a	-0.4819	1	2
17	ab	17a	-0.509	1	2
16	ab	16a	-0.5204	1	2
15	ab	15a	-0.5204	1	2
14	ab	14a	-0.5655	1	2
13	ab	13a	-0.5835	1	2
12	ab	12a	-0.6165	1	2
11	ab	11a	-0.6813	1	2
10	ab	10a	-0.6813	1	2
9	ab	9a	-0.8226	1	2
8	ab	8a	-0.8226	1	2
7	ab	7a	-0.9185	1	2
6	ab	6a	-11.3231	1	2
5	ab	5a	-11.3324	1	2
4	ab	4a	-11.3324	1	2
3	ab	3a	-11.3358	1	2
2	ab	2a	-11.3358	1	2
1	ab	1a	-11.3362	1	2

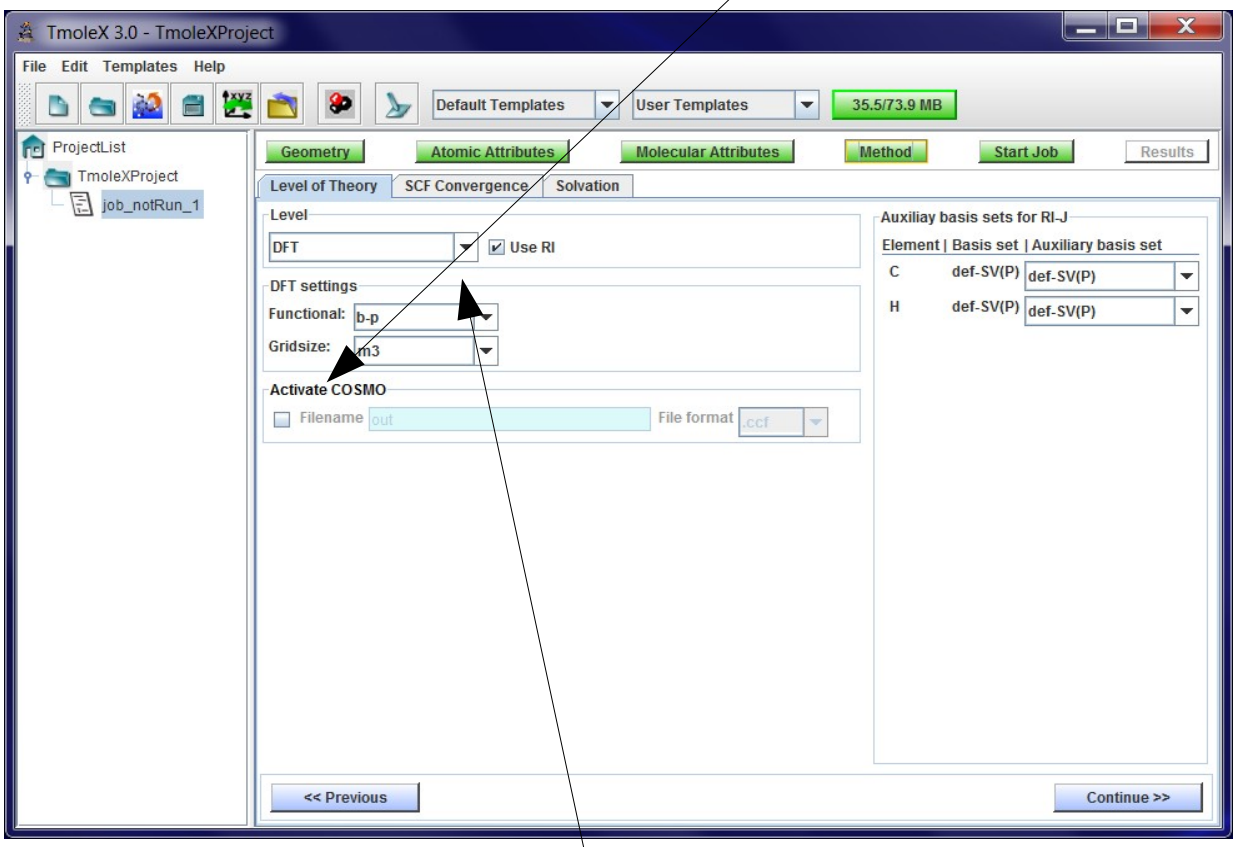
The default for the multiplicity is *automatic* – TmoleX will generate molecular orbitals by doing an Extended Hückel Guess and fills in the electrons according to the orbital energies. It will recognize closed and open shell cases and switches to restricted (RHF) or unrestricted (UHF) settings.

Note that you have to generate new orbitals if you change the multiplicity. In this case, i.e. multiplicity *not* set to automatic, will always result in unrestricted calculations!

In this panel you can also charge freeze core orbitals for correlated calculations, or switch on Fermi smearing. Switch from Table to Diagram to see the usual orbital occupation graphics. Use the left mouse button to set a freezing point for frozen core approximation settings, and the right mouse button to zoom in (or click once to zoom out).

2.5.4 Level of theory: Select method

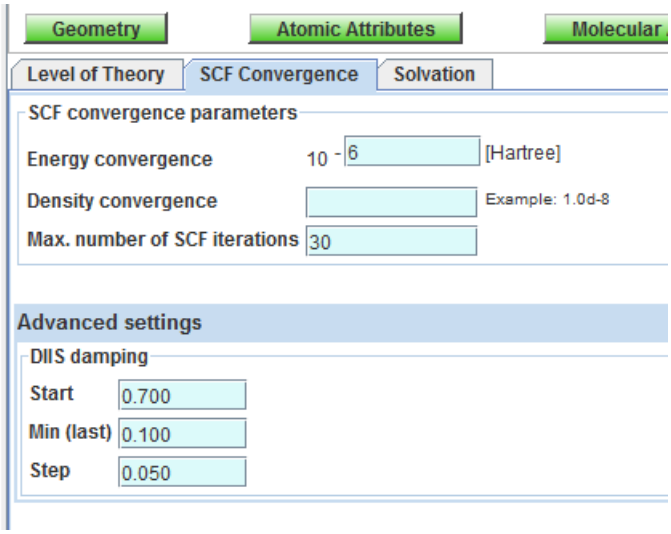
In the Method panel you can choose the level of theory, activate COSMO, select auxiliary basis sets, and advanced SCF settings can be changed.



The level of theory for your calculation can be set here. Currently nine different methods are available within TmoleX:

- Hartree-Fock
- DFT (with or without RI-J), RI-DFT is the default if you start a new session of TmoleX
- DFT + Disp, i.e. DFT with empirical dispersion correction (with or without RI-J)
- MP2
- CC2
- SCS-MP2 (spin-scaled MP2)
- SOS-MP2 (scaled opposite spin MP2)
- CCSD
- CCSD(T)

Settings for SCF convergence and special COSMO selections (recommended only for expert users) can also be found in the method section.



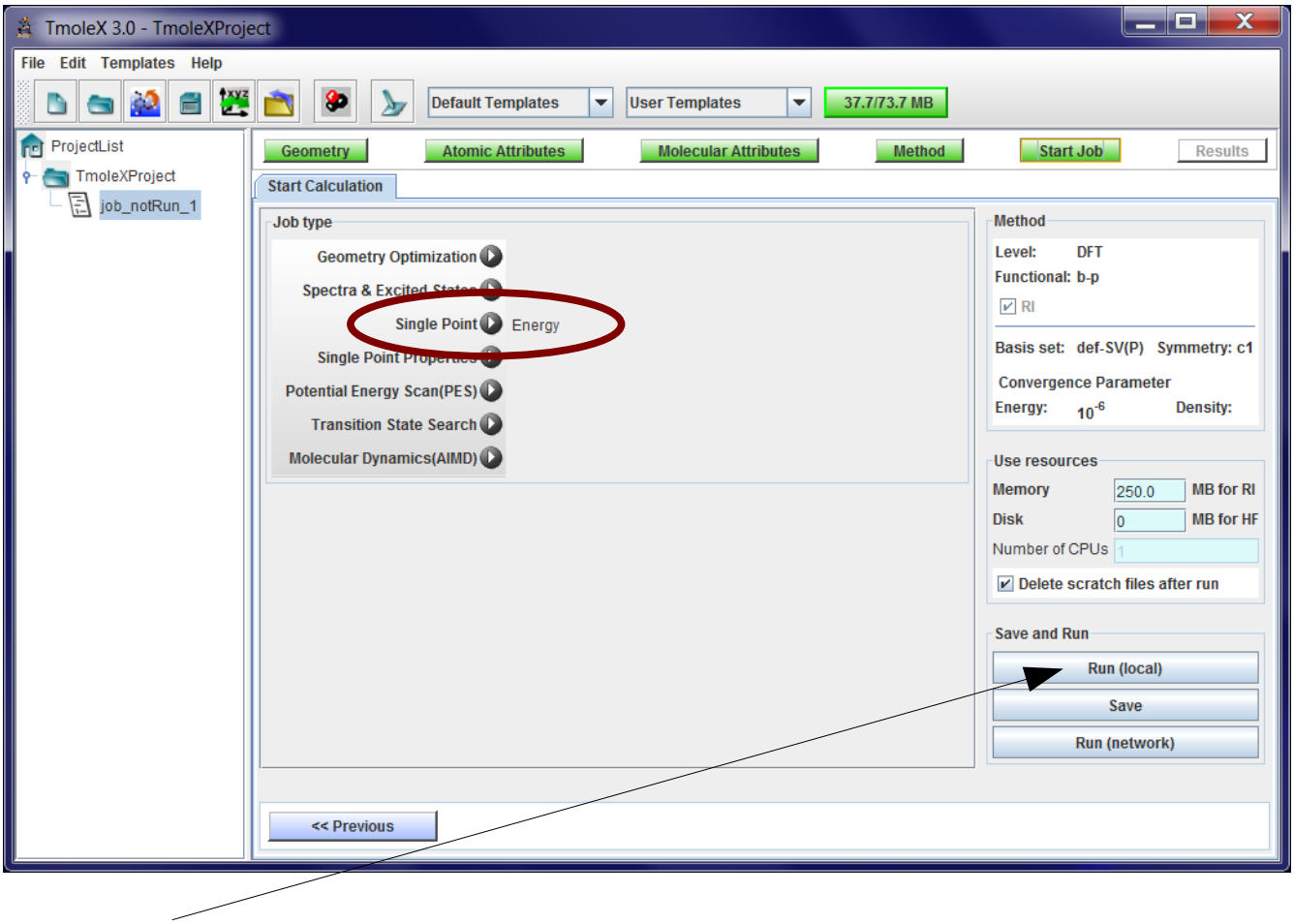
Energy and/or density convergence criteria can be entered in this panel. A density convergence criteria is useful for properties and methods that need a very accurate density like post-Hatree-Fock methods or TDDFT.

Note that the format of the parameters is different: The exponent has to be entered for the energy convergence while the density convergence threshold is a total number like 1d-8 (use `d` instead of `e` like `1e-8`, because TURBOMOLE reads them in as double precision number). This difference is due to the fact that the two corresponding TURBOMOLE keywords, `$scfconv` and `$denconv` in the control file are have to be given exactly like this – so TmoleX here tries to help to understand the default TURBOMOLE input.

Changing the default DIIS damping settings might be needed for complicated electronic structures like transition metal compounds. If the energy does not converge within many SCF iterations, the DIIS damping factors should be increased. See the TURBOMOLE manual for details about DIIS.

2.5.5 Start Job: Select kind of job and start it

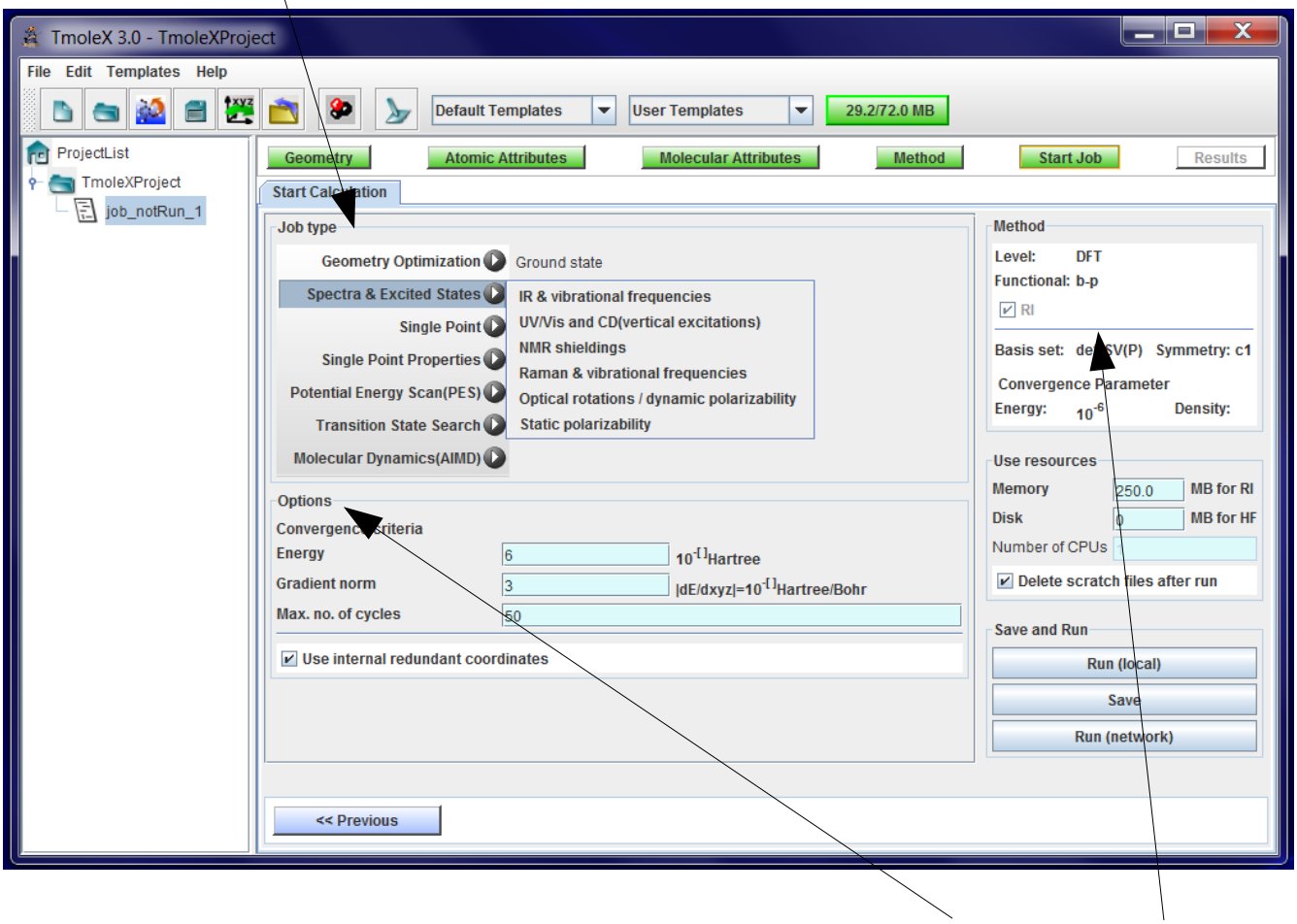
In the Start Job panel, a **single point energy** calculation can be started.



'Run (local)' will start the calculation in the present directory. 'Save' writes the complete input to disk for further use on the command line or later usage if needed. 'Run (network)' starts the calculation on a remote Linux/Unix computer, see chapter 7.

2. A quick tour

Click through the Job type options to see what kind of jobs are supported by TmoleX.

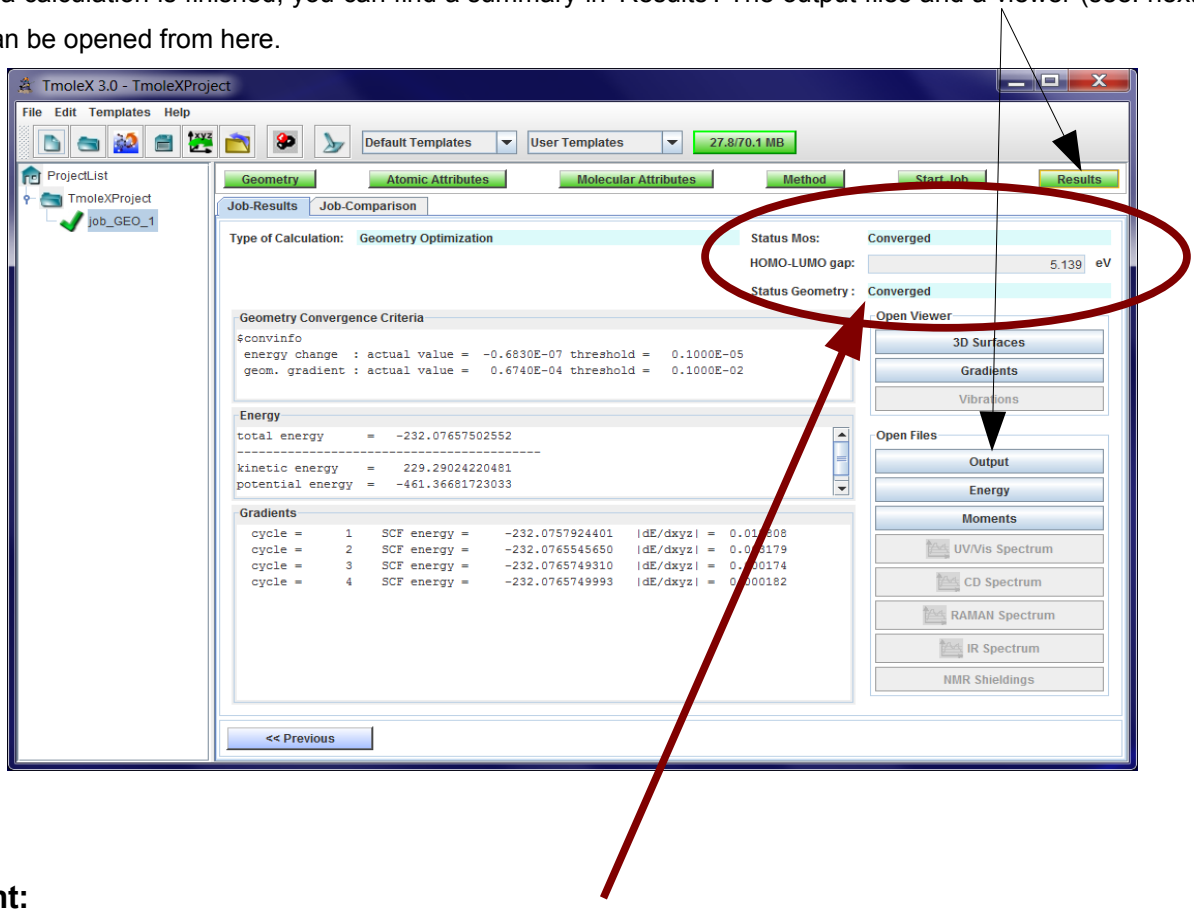


Depending on the job type, different options for the chosen job are displayed in the Options section. The Method section briefly summarizes the settings done in the four menus before (method, symmetry, basis set, etc.).

Finally, the 'Use resources' part can be used to set (maximum) amount of memory (RAM) and disk space for the calculation. If and how important those settings are depends on the method and job type. For ground state single-point energies and geometry optimizations at Hartree-Fock or DFT level, neither more memory nor more disk space will speed up the calculation significantly. For vibrational frequencies (IR and Raman spectra), post-Hartree-Fock methods or excited state calculations, more memory can improve efficiency a lot. Please note that the given memory value is *not* the total amount of RAM the program will use, just the parts that can be adjusted. Hence, do not enter more than roughly 80% of your total memory here to avoid huge performance problems!

2.5.6 Results

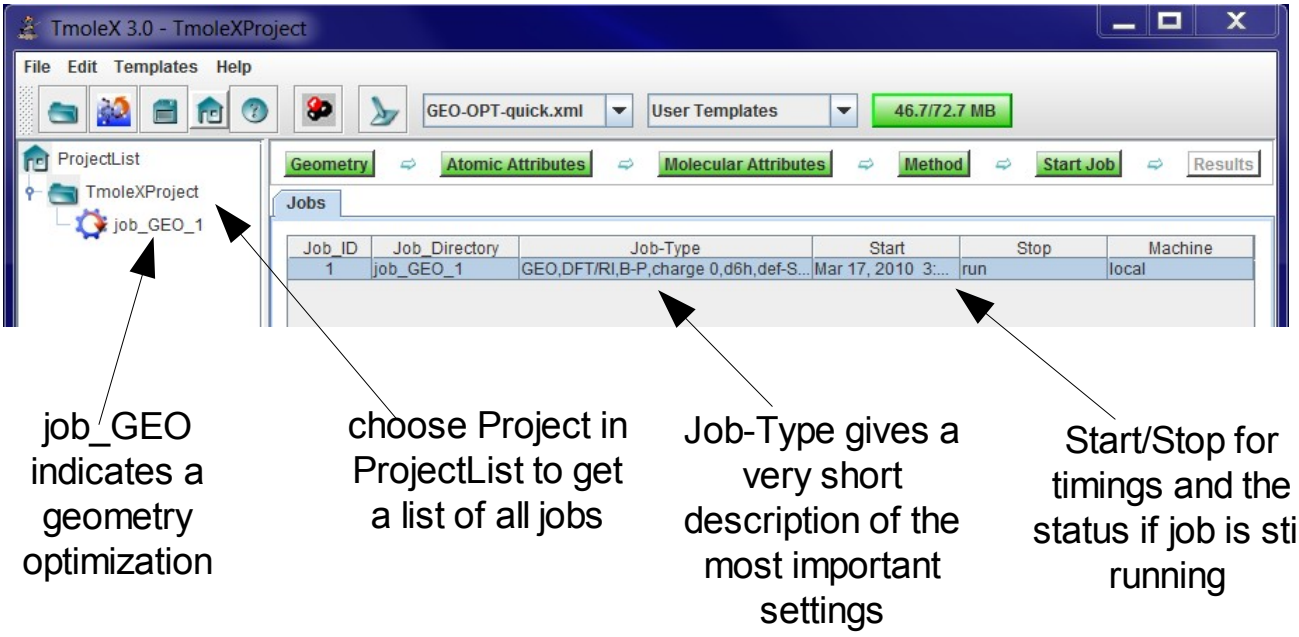
Whenever a calculation is finished, you can find a summary in 'Results'. The output files and a viewer (see. next chapter) can be opened from here.



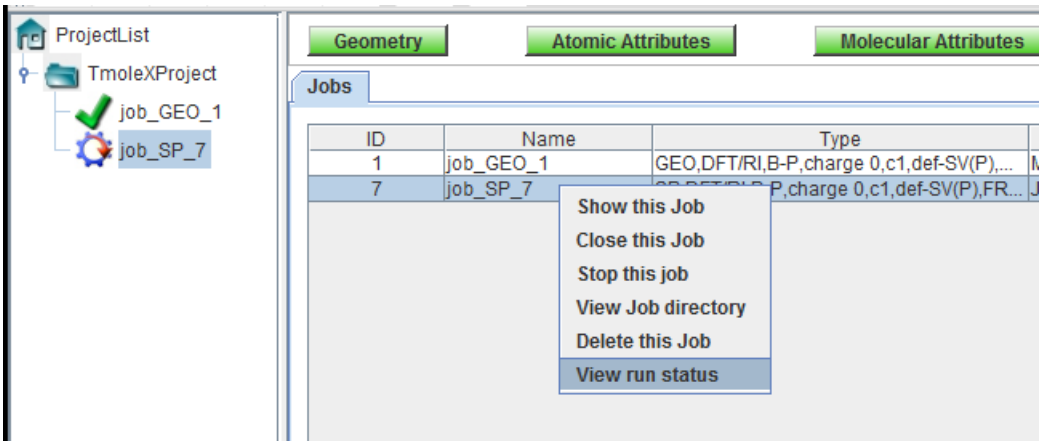
Important:

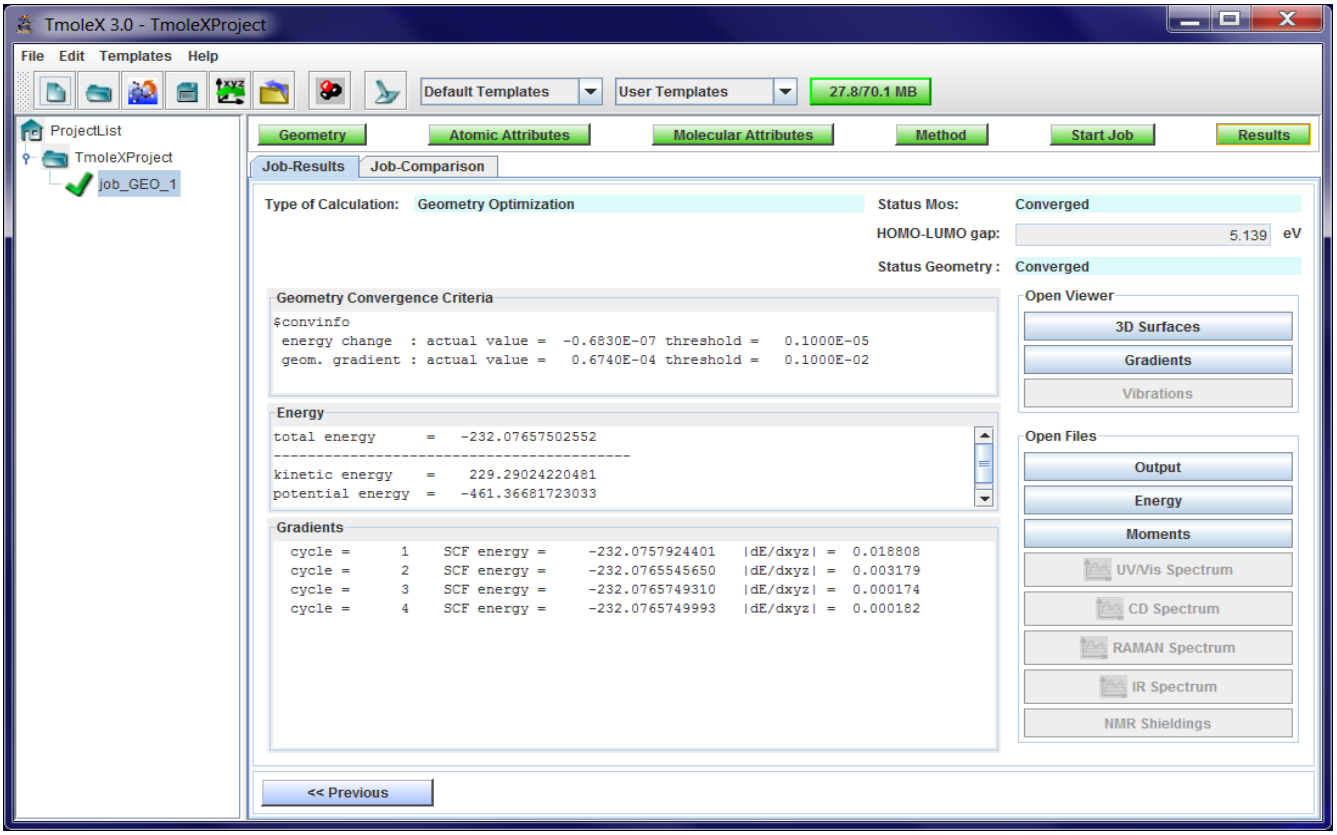
- Check the Status of the molecular orbitals and the status of the geometry optimization!
- In case that the orbitals (MOs) are not converged, restart the job – perhaps more SCF iterations or higher DIIS damping is required (see Method section)
- If the geometry is not converged, restart the optimization allowing more geometry cycles.
- Also make sure that the HOMO-LUMO gap is positive. Otherwise you have a hole in the occupation (which might be what you want, but usually this should not be the case), and you did not get the proper ground state of the electronic structure.

2.6. Job Administration



Click on the name of the Project in the ProjectList and use the right mouse menu in the 'Jobs' section to close (remove just from the list, let all files on disk), stop (stop running jobs, let files on disk), delete (delete job from the list and delete the files from disk) jobs. 'View Job directory' will open the default file browser on your system with the directory where the selected job is running or was running. 'View run status' can be chosen for running jobs (not remote jobs without a queuing-system, for remote jobs which run under a queuing-system, the status of the queue is shown).





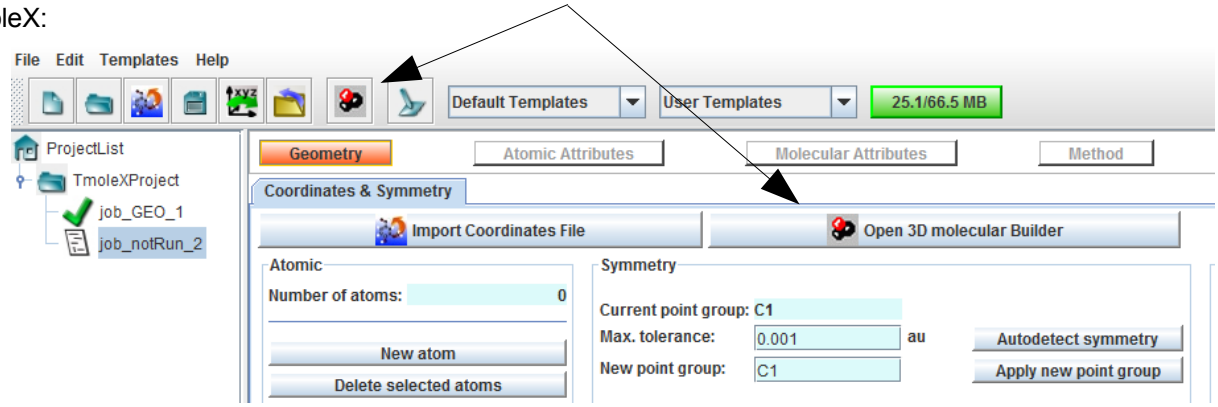
The progress and status of all calculation belonging to your project, which are currently running or ran before, can be accessed via the “Job-Administration” by clicking on the project name *itself* instead of a job within the project. After starting a first job, you can instantly set up and even launch a new one. For performance considerations you will however prefer running only one job at a time in most cases.

Note: TmoleX does not yet cover all possible kinds of calculations and input options that TURBOMOLE offers. If you need additional options but want to use TmoleX, you can manually edit the control file. Please refer to the TURBOMOLE manual for further information.

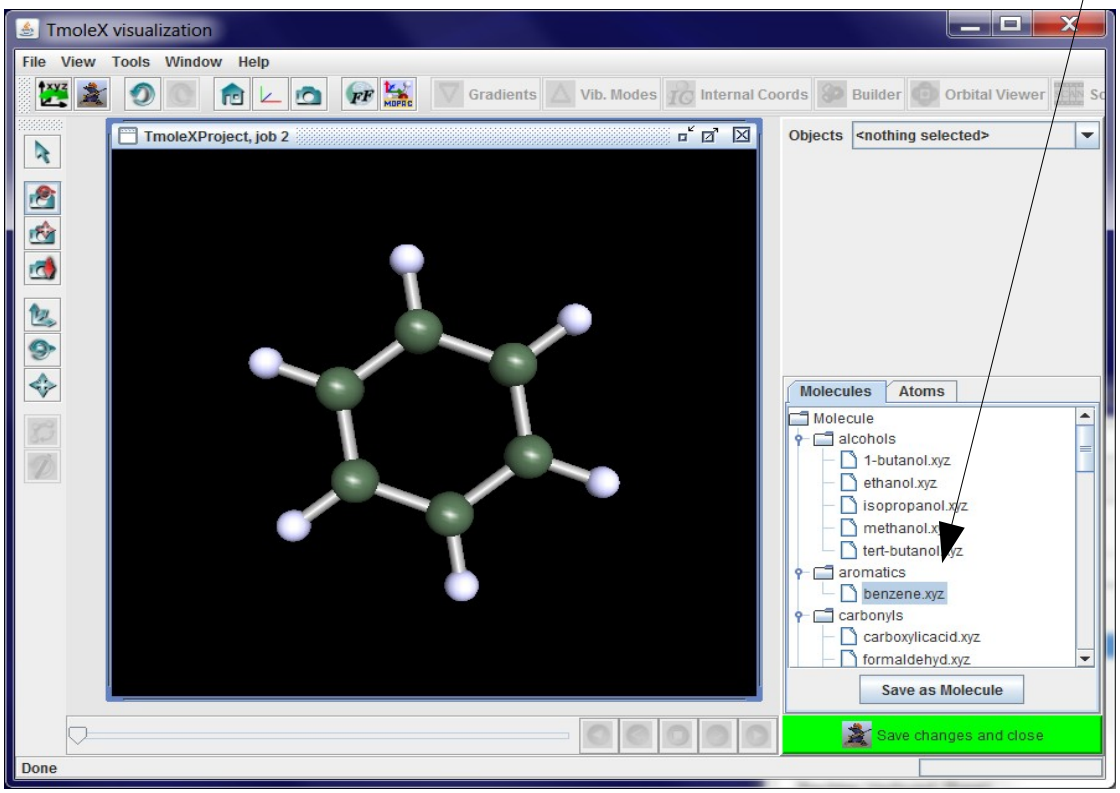
3. The 3D visualization

3.1. The builder

To open the molecular builder click on either the button in the tool bar or the button in the Geometry panel of TmoleX:



The molecule builder can be used most conveniently by starting from fragments and modifying these. Double-click on a fragment to import it in the builder.



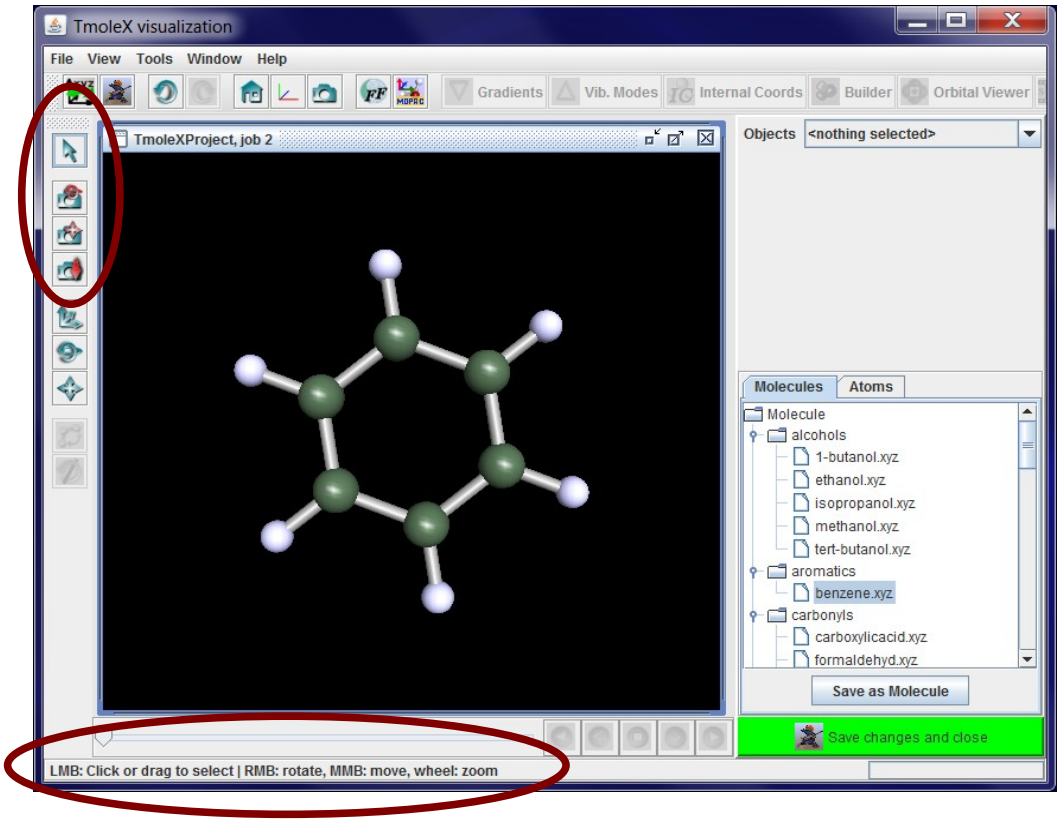
3.1.1 Navigation

Left mouse button or or q on the keyboard: *Select*

Right mouse button or : *Rotate view*

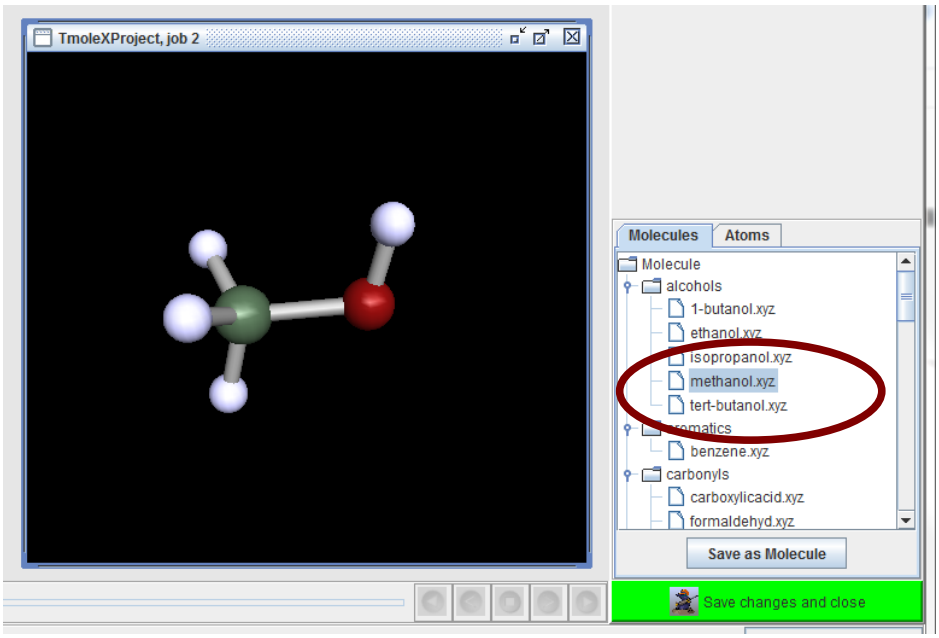
Middle mouse button or : *Move*

Scroll wheel or : *Zoom*

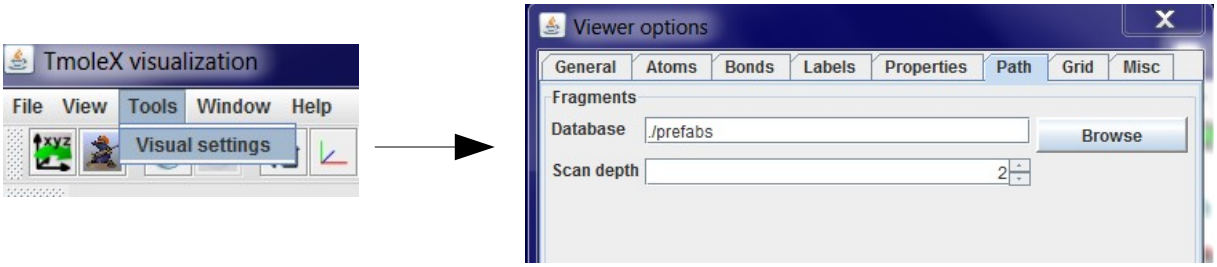


3.1.2 Pre-stored structures

There are different ways to add molecules and fragments which build up a structure.
Double-click or drag-and-drop molecules from the Molecules section on the right to the window:



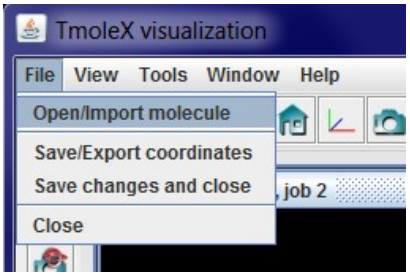
The molecules in the right part of the window are by default taken from the *prefabs* directory of the TmoleX installation. This can be changed to a user-defined directory in the Tools → Visual settings menu:
The files are stored in standard xyz format, the second line can contain the name of a fragment with the



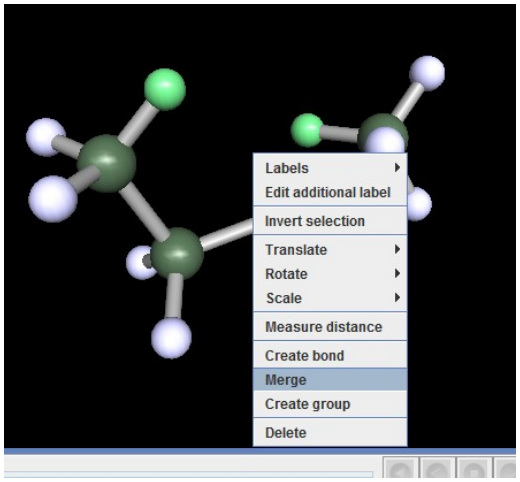
definition of the number of atom which can be replaced (see the files in the TmoleX/prefabs directories).
The 'Save as Molecule' button can be used to store the structure that is visualized in the 3D window to the users data base. The atom that is selected when saving is the one that will be replaced when using the 'Substitute with...' option in the right mouse panel (see below).

3.1.3 Import structure

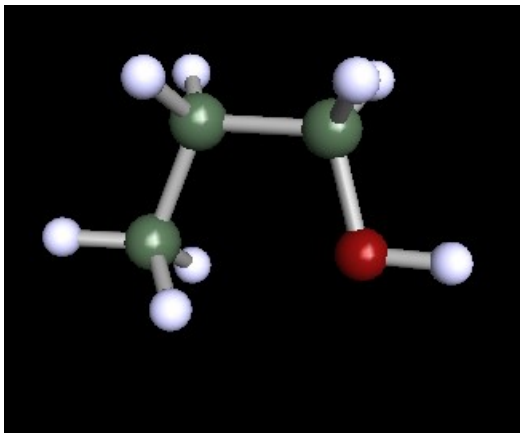
Instead of building a molecule from scratch, an existing molecule in different formats (sdf, ml2, xyz, cosmo, …) can be imported using the File/Open menu entry within the visualizer.



This structure can then be used for modification or being saved in the user data base as described above. Another possibility is to load two or more molecules and select one atom of two different fragments:

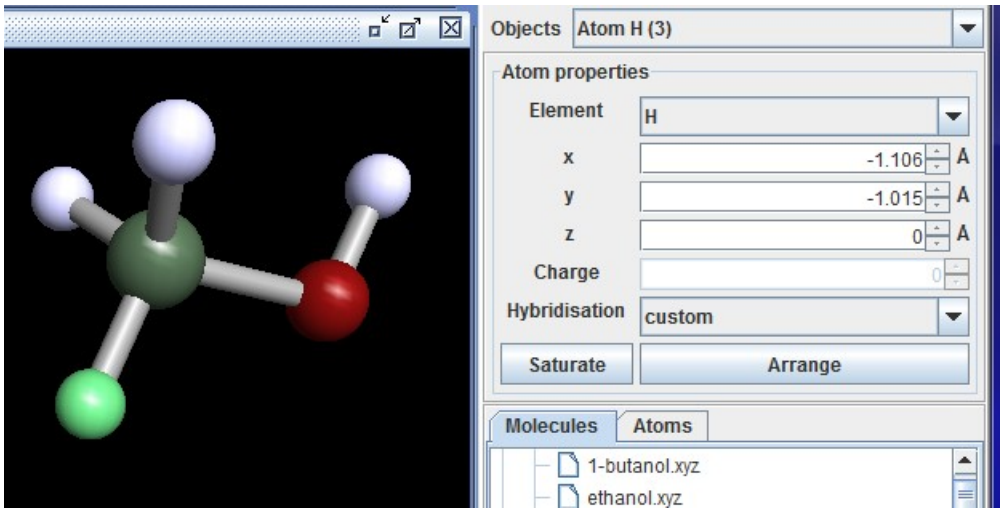


Use the right mouse button and select the *Merge* option. TmoleX will join the two fragments and re-arrange the resulting structure such that the overlap of the atoms is minimal:

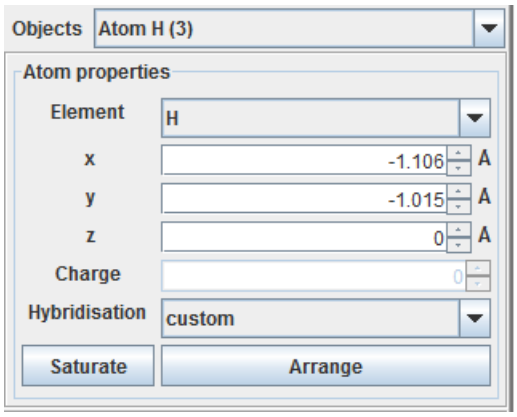


3.1.4 Building step by step 1

Change to selection mode (q or ESC key or arrow button on the left side) if you are not already in this mode.
Select an atom:

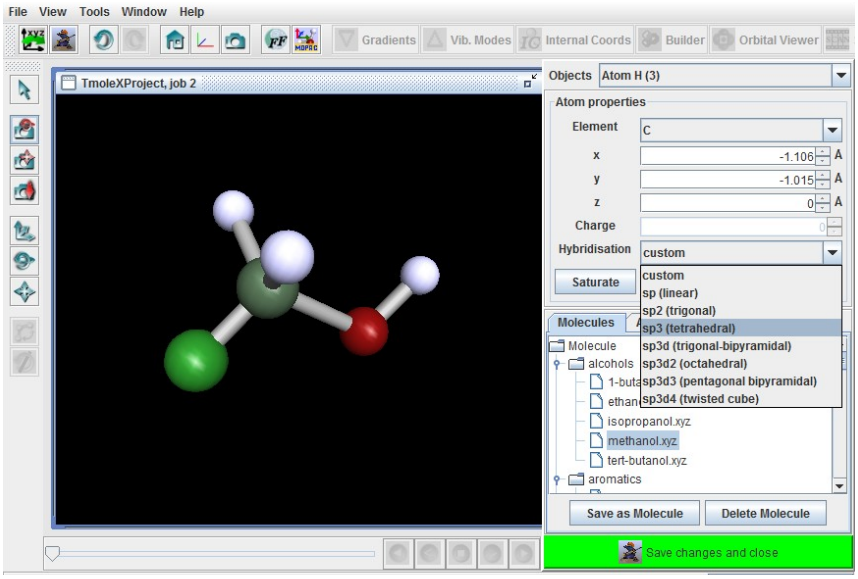


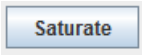
On the right side the properties of the selected item (atom, bond, measure, etc.) are shown.
For objects which are hard to select with the mouse, the Objects chooser can help since it contains all displayed objects, including measurements and constraints.



Most entries can be changed in the fields.

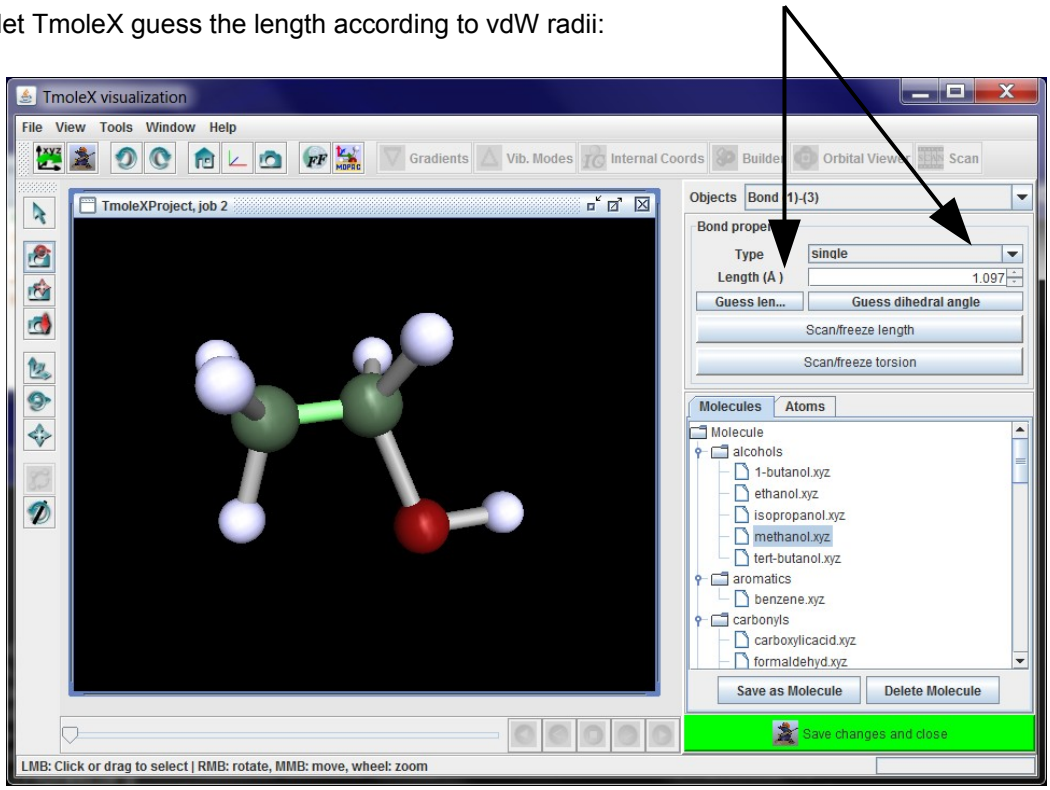
Change the Element from H to C and also the Hybridisation to sp3:



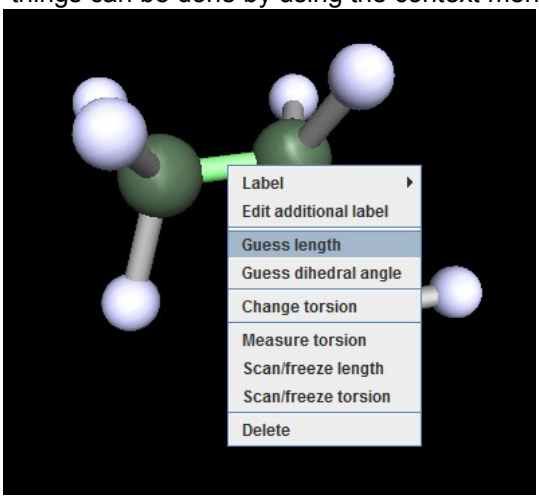
Next, click on  to add missing hydrogens to the selected atom according to the given hybridisation.

3.1.5 Change bond length

Now the bond length to the newly created methyl group is too short, so select the bond and either enter a new value or let TmoleX guess the length according to vdW radii:



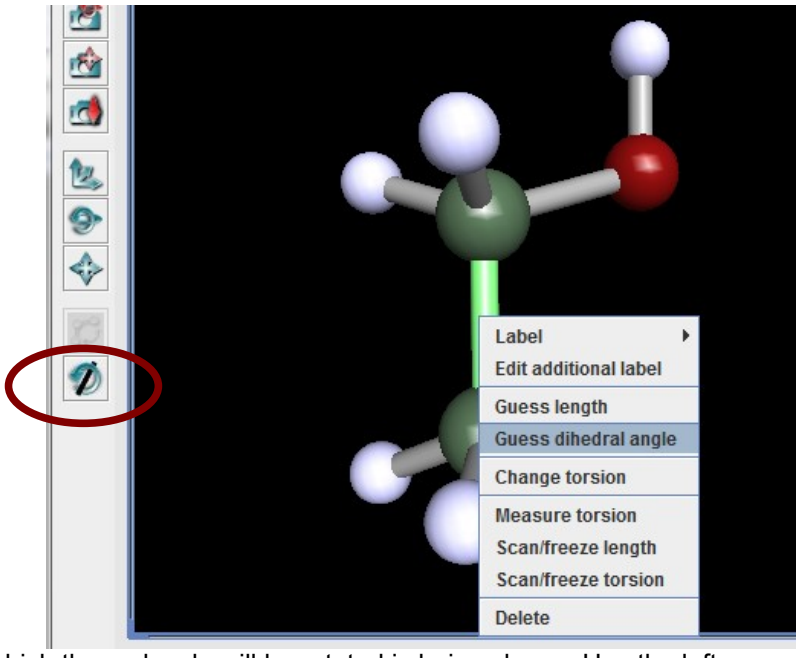
The length and also many other things can be done by using the context menu of the right mouse button:



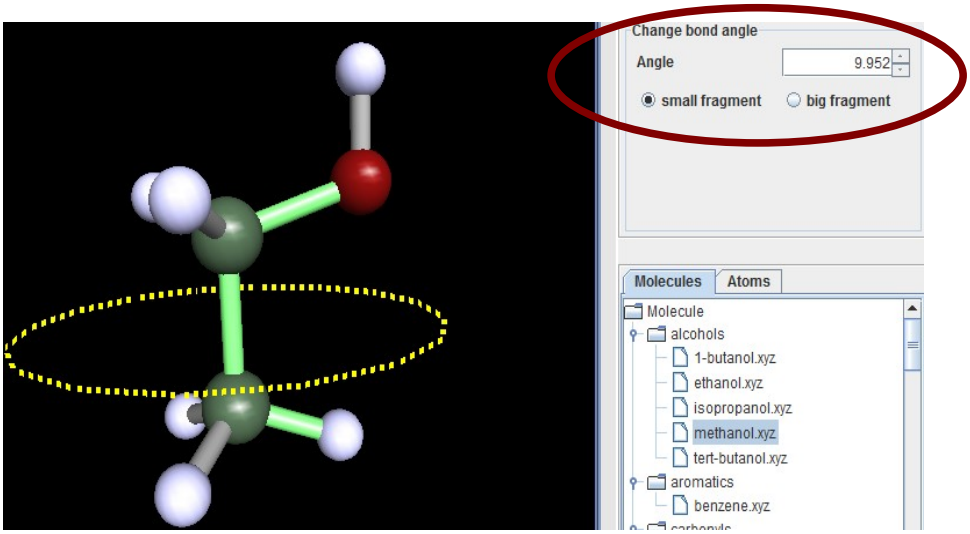
Hint: If you want to change a bond length (or an angle or torsion) and there are no bonds to select, simply add a new bond between two selected atoms using the right mouse menu.

3.1.6 Change torsion

To **change the dihedral angle**, click on the middle bond or select three bonds (holding shift key will add selections) which define the angle and then either use the button on the left that will show up or again the right mouse menu:

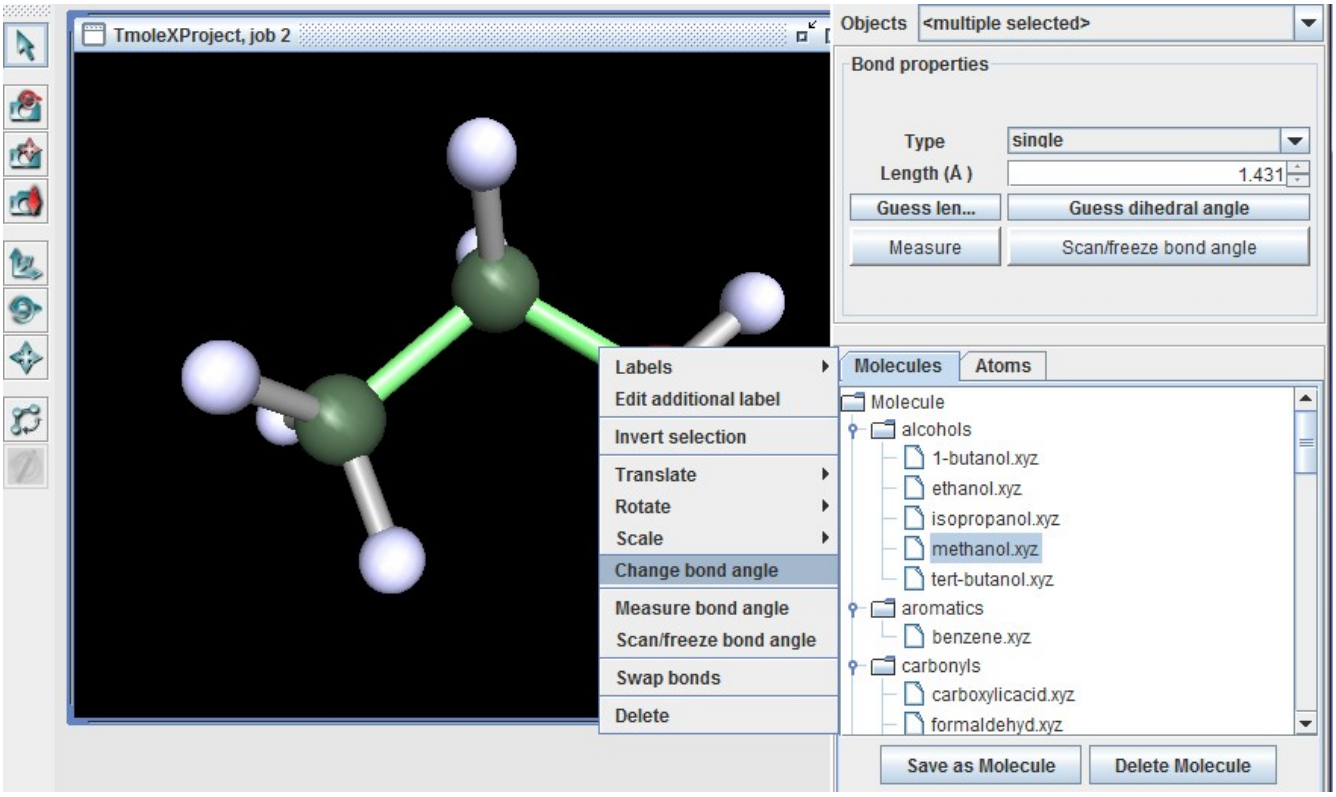


The torsion around which the molecule will be rotated is being shown. Use the left mouse button to change the angle – moving to right or up will increase the value, moving the mouse to the left or down will decrease the angle. The value of the angle can be entered directly on the right side, and one can also choose if the smaller or the bigger fragment is being moved.



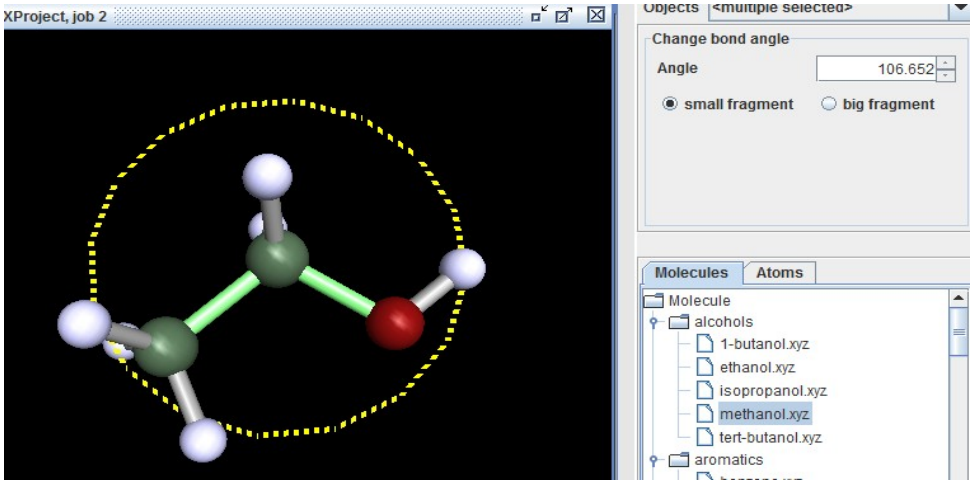
3.1.7 Change bond angle

To **change a bond angle**, select two adjacent bonds (shift-click for the second one) and either click on the button on the left side or use the right mouse button to change the value:



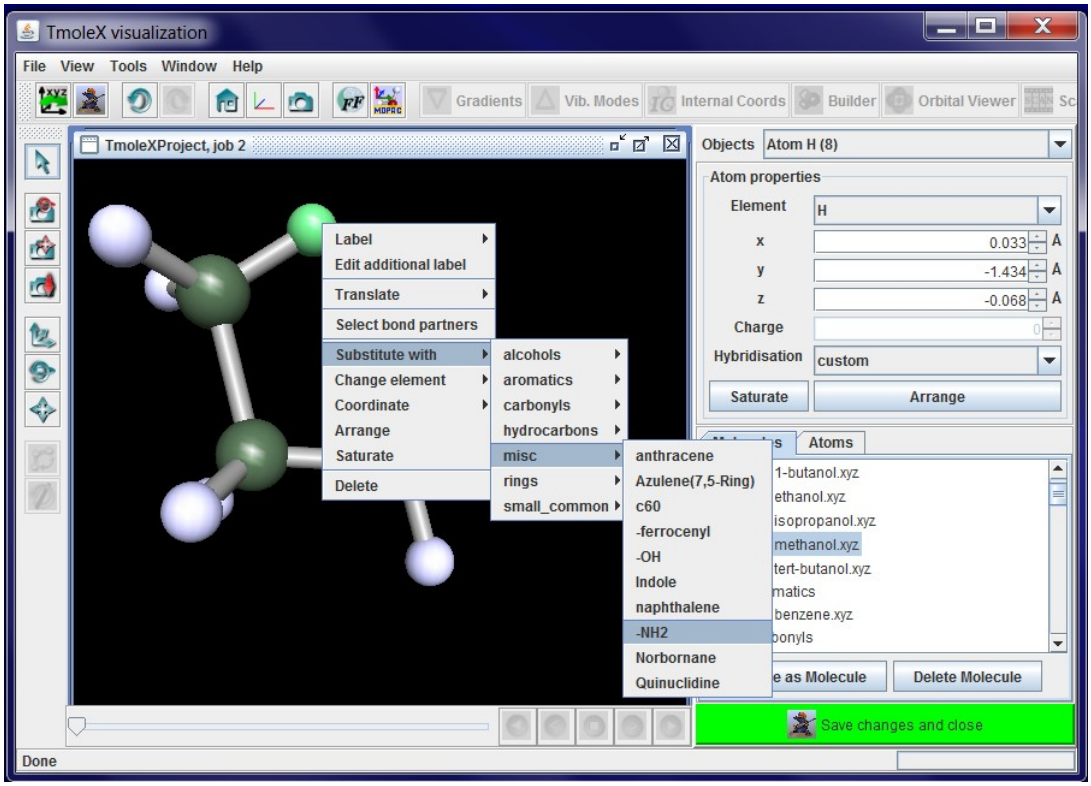
The properties of the angle are shown and can either be changed by clicking on the left mouse button and dragging the mouse or by editing the field:

Like for torsional angles, the small and big fragment option decides which part of the molecule is being moved.



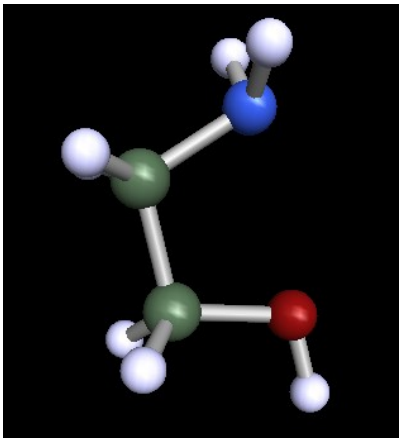
3.1.8 Building step by step 2

Instead of changing an atom to a different element, to change hybridisation and use the saturate option, an atom can also be replaced by a pre-stored fragment.



Select an atom, use the right mouse button and click on 'Substitute with'.

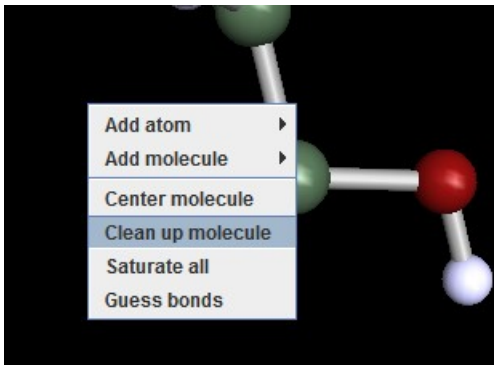
Note: The fragments that are shown are the molecules of the user data base (or the default pre-stored molecules after installation as shown here). When saving molecules to this data base, it is possible to select an atom when saving. This selected atom of the stored fragment is the connecting atom.



3.2. Preoptimization

There are three options to pre-optimize a guess structure:

- Unselect all objects by clicking on the background
  Use the right mouse button and select:

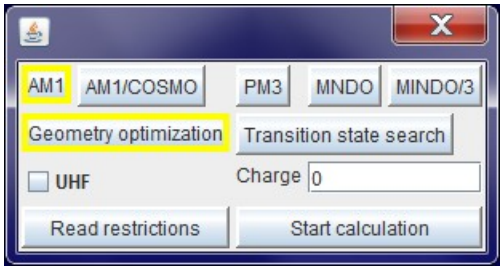


  A simple rearrangement which minimizes the overlap of the van-der-Waals radii of all atoms

- UFF – a universal force field as implemented in TURBOMOLE can be used by clicking on the FF button:

- The recommended way is to use MOPAC7, which is included in the default installation of TmoleX.

  The MOPAC7 button will open a new window with several options.



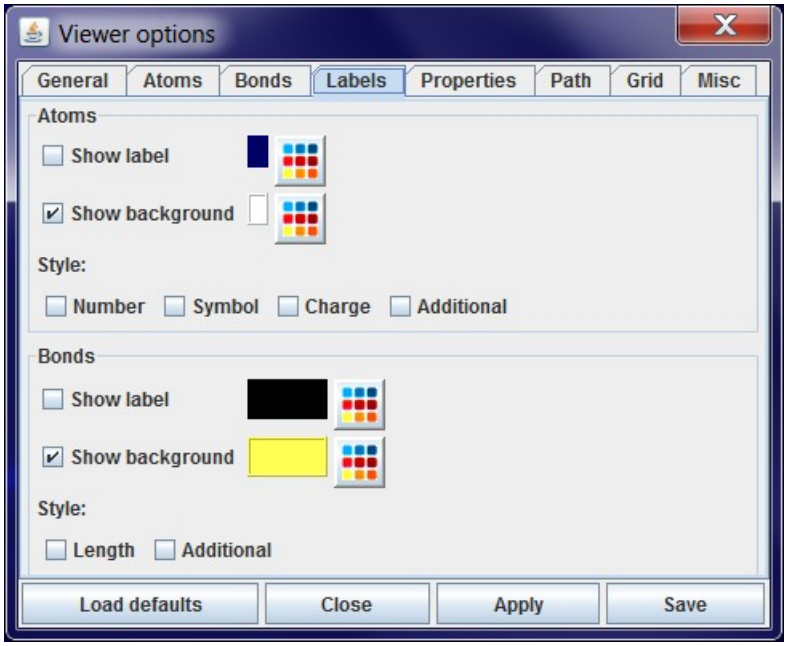
  AM1, PM3, MNDO, MNDO/3 are the available methods (they all are parametrized for a certain number of elements). AM1/COSMO is the default setting for COSMOtherm input files at BP-SVP level (first do a geometry optimization at this level and then a single-point DFT calculation with COSMO and SVP basis set). Unrestricted calculations can be done with UHF, guess structures for transition states can also be searched. A molecular charge has to be entered to calculate ions.

3.3. Labels and Measurements

Labels for atoms and bonds as well as measures of lengths and angles can be switched on or off for the complete structure or individually for each object.

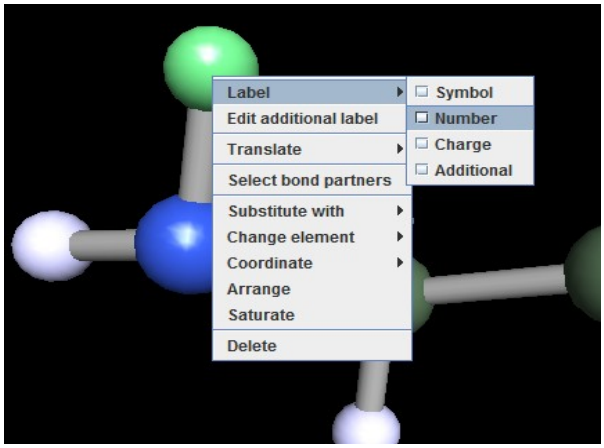
- Display labels for all atoms or bonds

  In the 3D viewer select Tools → Visual settings and switch to the Labels section:



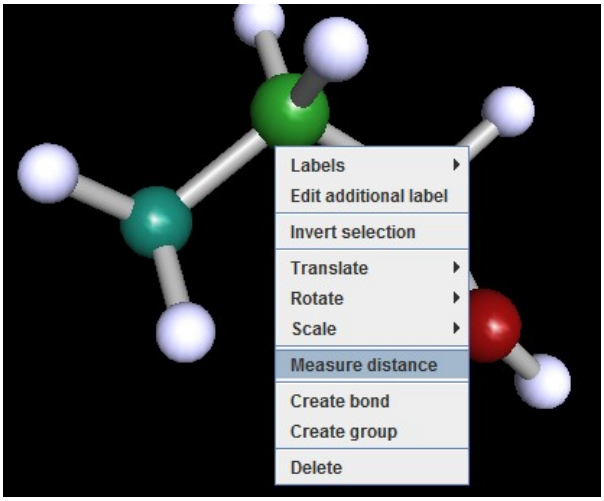
  For atoms the atom number, the element symbol, the charge and additional text (which can be entered by the user with the right mouse button menu within the viewer window) can be displayed. Depending on the background colour and the colour of bonds and atoms the labels can be hard to read. The background settings here refer to the background of the text field only.

- To display labels of one or several atoms/bonds only, use the right mouse menu:

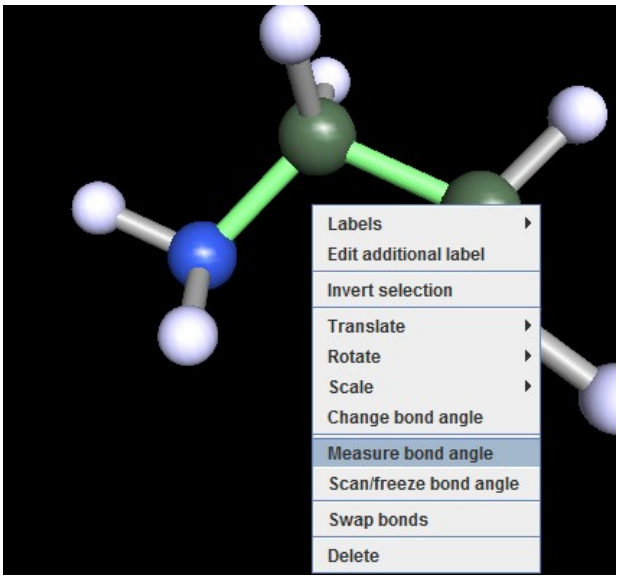


Own text can be entered in the second item of the right mouse menu. To add or remove labels for several atoms or bonds, just select several items and then use the right mouse button for the selection.

- Measures can be added with the right mouse menu, what is measured depends on what you have selected:
  - select two atoms: measure distance



  - select two bonds: measure angle



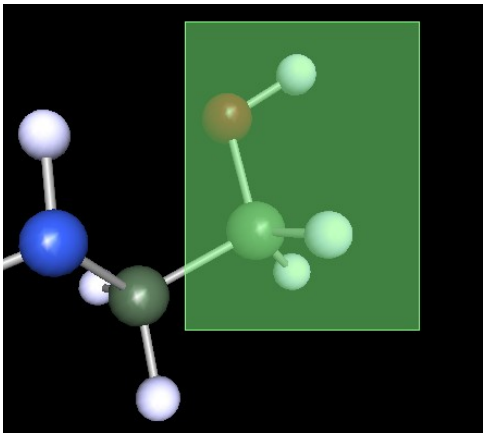
  - select three bonds: measure torsion...

Measures can be selected and deleted with the Measures pull down list:

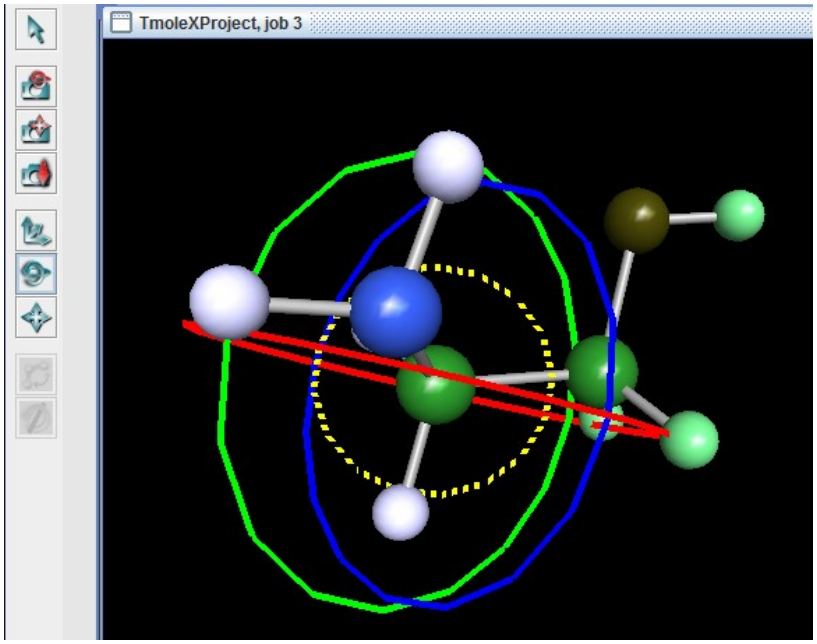
3.4. Moving, Rotating, Scaling

It is often helpful to move or rotate parts of the molecule to a new position. This can be done within TmoleX with several powerful possibilities, but the usage is not self-explaining. So here are the options:

- Select several atoms,

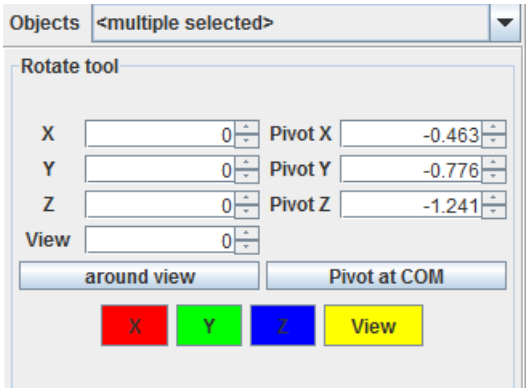


hold shift key and select the atom around which the rotation shall be done. **The last atom that is selected will be by default the centre of the rotation!** Use the right mouse menu or the button or the key 'e' to switch to rotation mode.



Rotation of the selected atoms can be done using x,y,z axis as rotation axis. In addition to that, the yellow circle indicates the rotation around the axis that is perpendicular to your screen – at the moment you activate the rotation mode. Use the right mouse button to rotate the view, the middle mouse button to move the camera and the scroll wheel for zoom. Those mouse movements will not change the coordinates, just the view.

To rotate around x,y, z, or the initial view direction, use the left mouse button and drag the mouse.



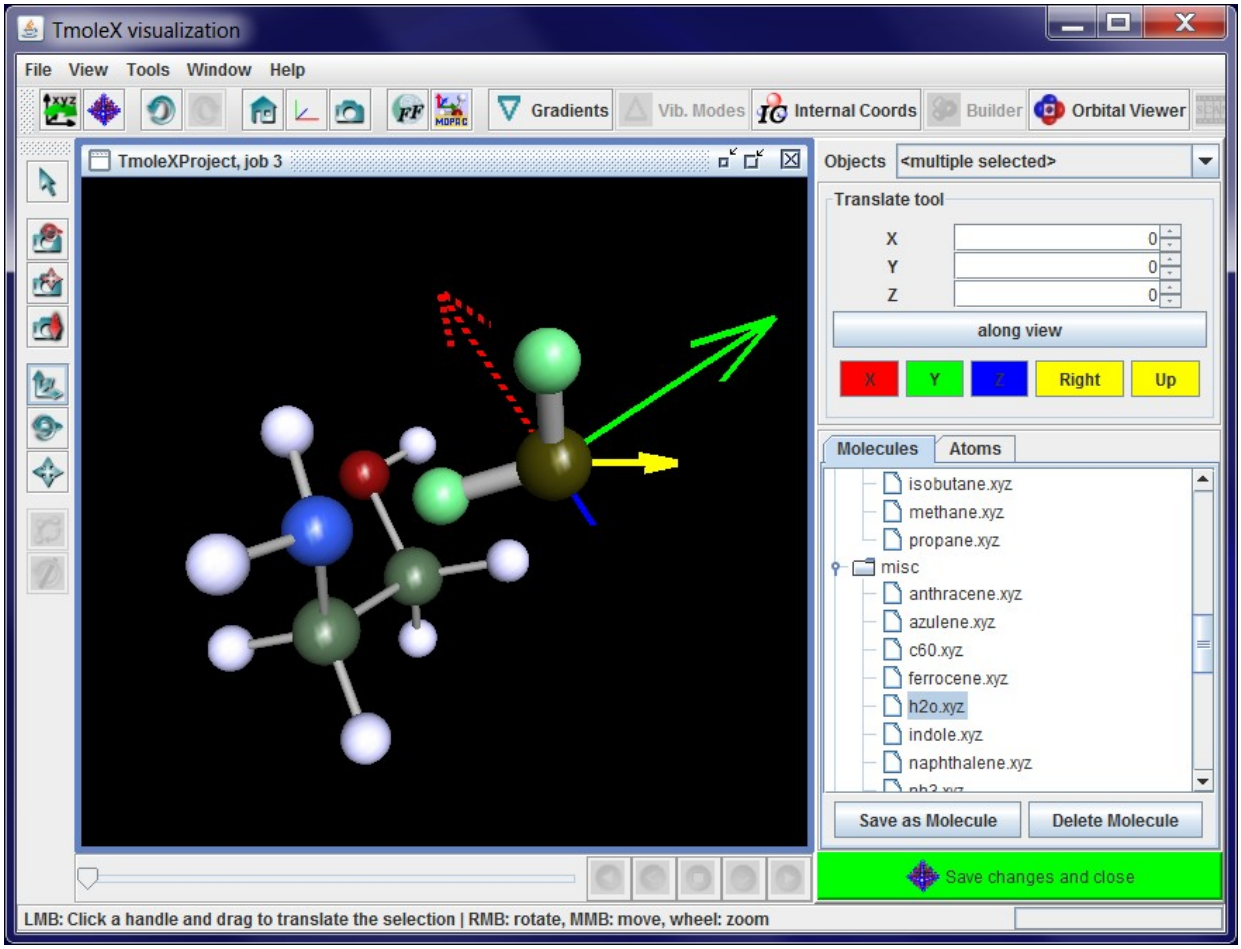
Use the coloured buttons on the right side of the window to switch the rotation axis, or click directly on the coloured circles.
The 'around view' button will reset the yellow 'view' rotation axis to your current viewing direction. Note that rotating the view with the right mouse button does not change the rotation axis!
The 'Pivot at COM' changes the centre of the rotation to the centre of mass of the selected atoms.
Rotation angles can be entered (in degrees) to the corresponding X,Z,Y, View fields. The center of rotation, i.e. the pivot, can also be entered manually if needed.

Note that the selected atoms which will be rotated do not have to be connected.

- Moving atoms or fragments is very similar to the rotation procedure described above. Select the atoms that shall be moved and use the right mouse menu (Translate), or the button , or press the key 'w'.

Hints:

- Double-click on an atom to select the whole fragment (all atoms that are connected by bonds).
- There is an option 'Select bond partners' in the right mouse menu which extends the selection around each already selected atom to its next (bonded) neighbours.



Again, change the direction of movement either by clicking on the coloured buttons on the right side, or by clicking on the coloured arrows.

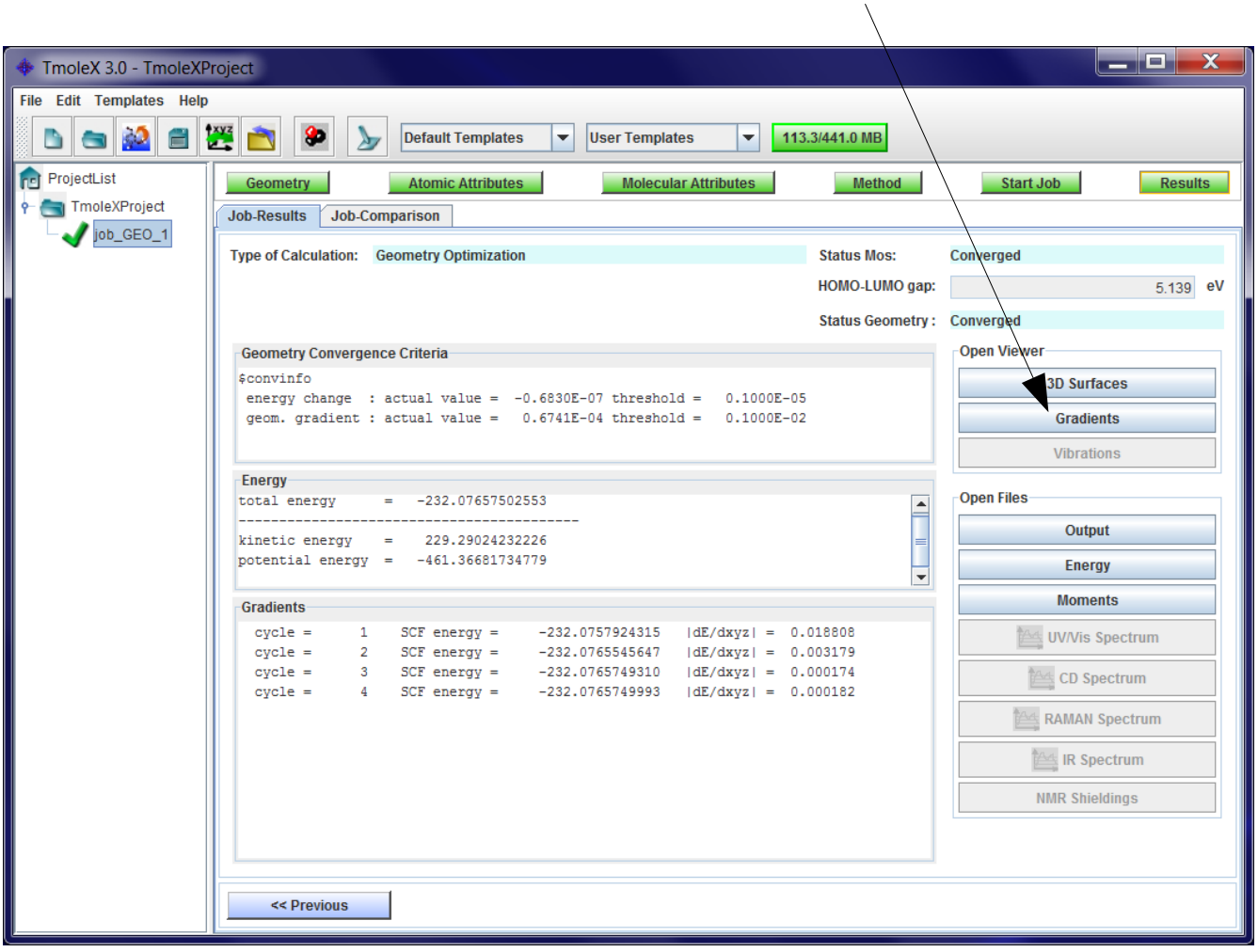
Note:

- Holding the left mouse button and moving the mouse to the *right or up* will move along the *positive direction* (plus x,y,z values), and moving the mouse *down or to the left* will *decrease* the coordinates – not matter from which direction you are looking at the structure! This can sometimes lead to the fact that moving for example the mouse to the left will move the fragment to the right (because you are looking at the structure from 'behind').
- Again, in addition to the absolute directions x,y,z, you can move the selected atoms along the direction that corresponds to the 2D coordinates of your screen: Right/Left and Up/Down. Click on 'along view' to reset the Right and Up direction to your current view on the structure.

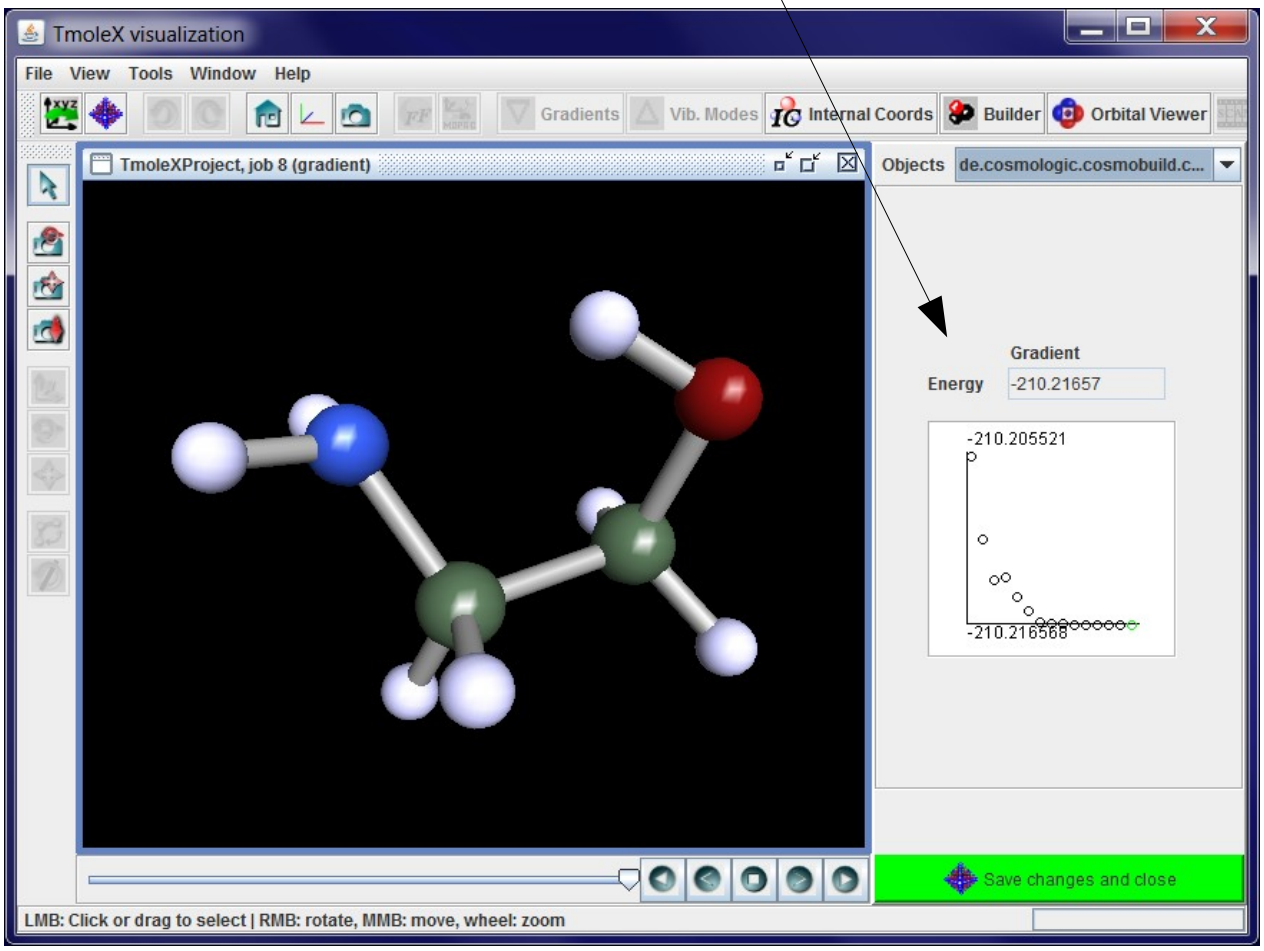
- Finally, the scale tool (key 'r') scales or resizes relative distances between atoms. Add a benzene ring, select it, and use this tool to see what it does.

3.5. The gradient viewer

Once you have completed a geometry optimization, you can open the gradient viewer from the results panel.



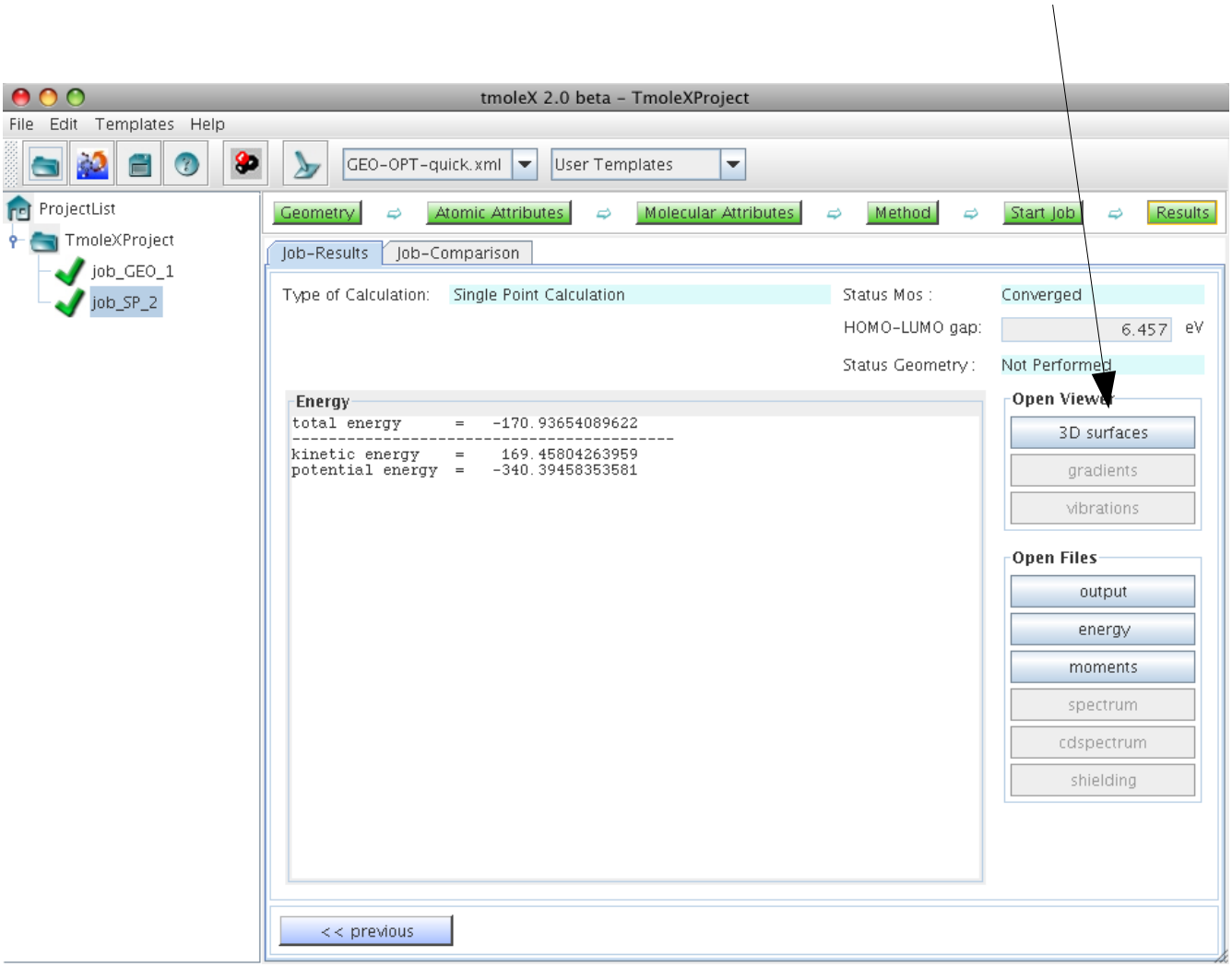
The total energies for the optimization steps can by viewed here.



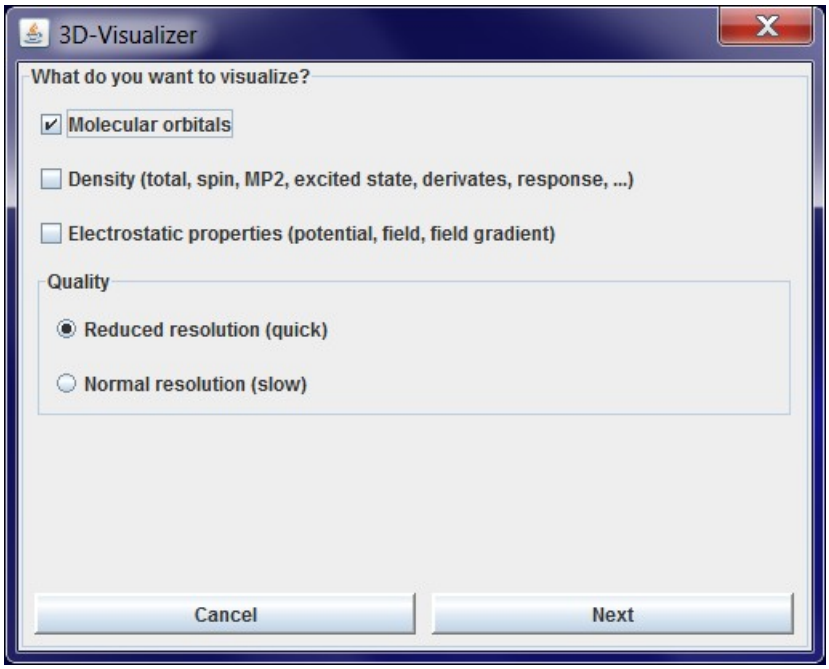
The different geometry can also be viewed as a movie by using the play buttons or moving the slider. The smaller < and > go stepwise back and forth.

3.6. Surface plots

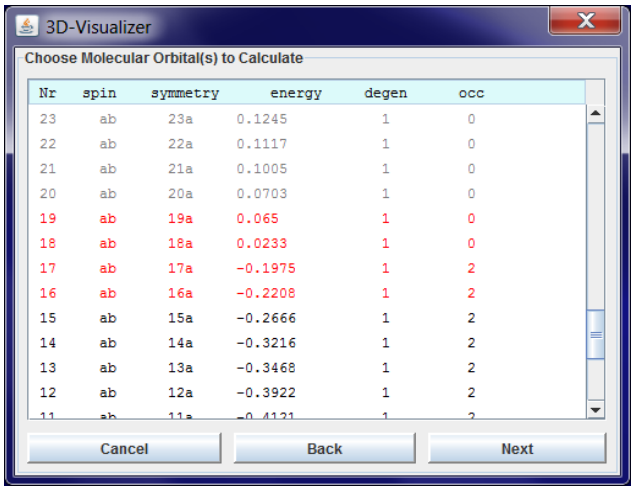
Once you have converged molecular orbitals, TURBOMOLE offers the possibility to write different properties on a grid for a visual post-processing. This is reproduced in TmoleX interactively starting from '3D surface'.



In a following window you will be asked which property to calculate. By default the quality is set to quick. Please note, that the calculation in normal resolution might take quite some time.

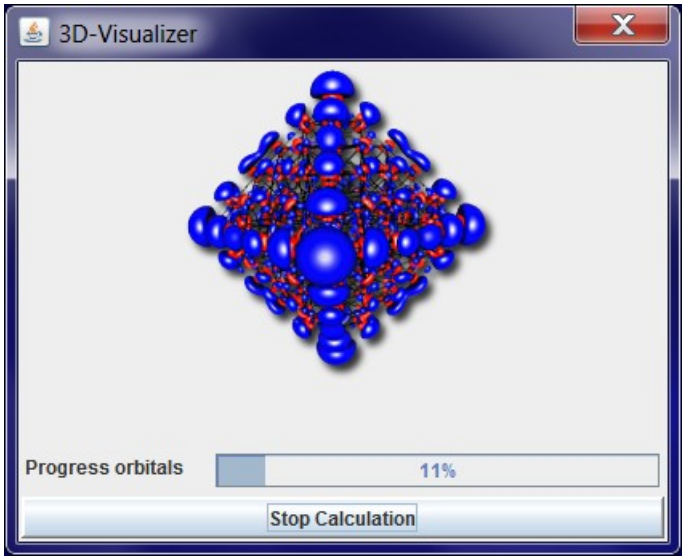


For most users the molecular orbital will be of most interest. Select occupied or unoccupied orbitals and proceed with 'next' to the calculation. Hold <Shift> or <Control> key to mark a list of orbitals.



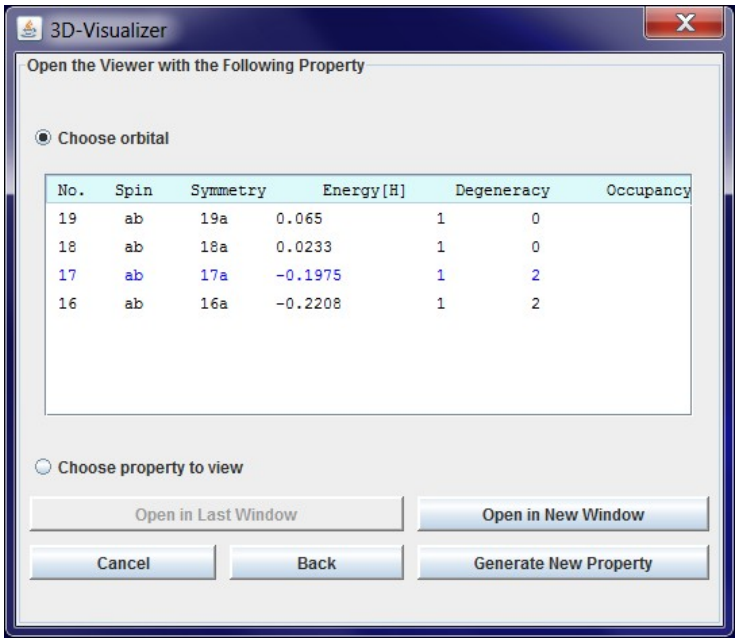
3.The 3D visualization

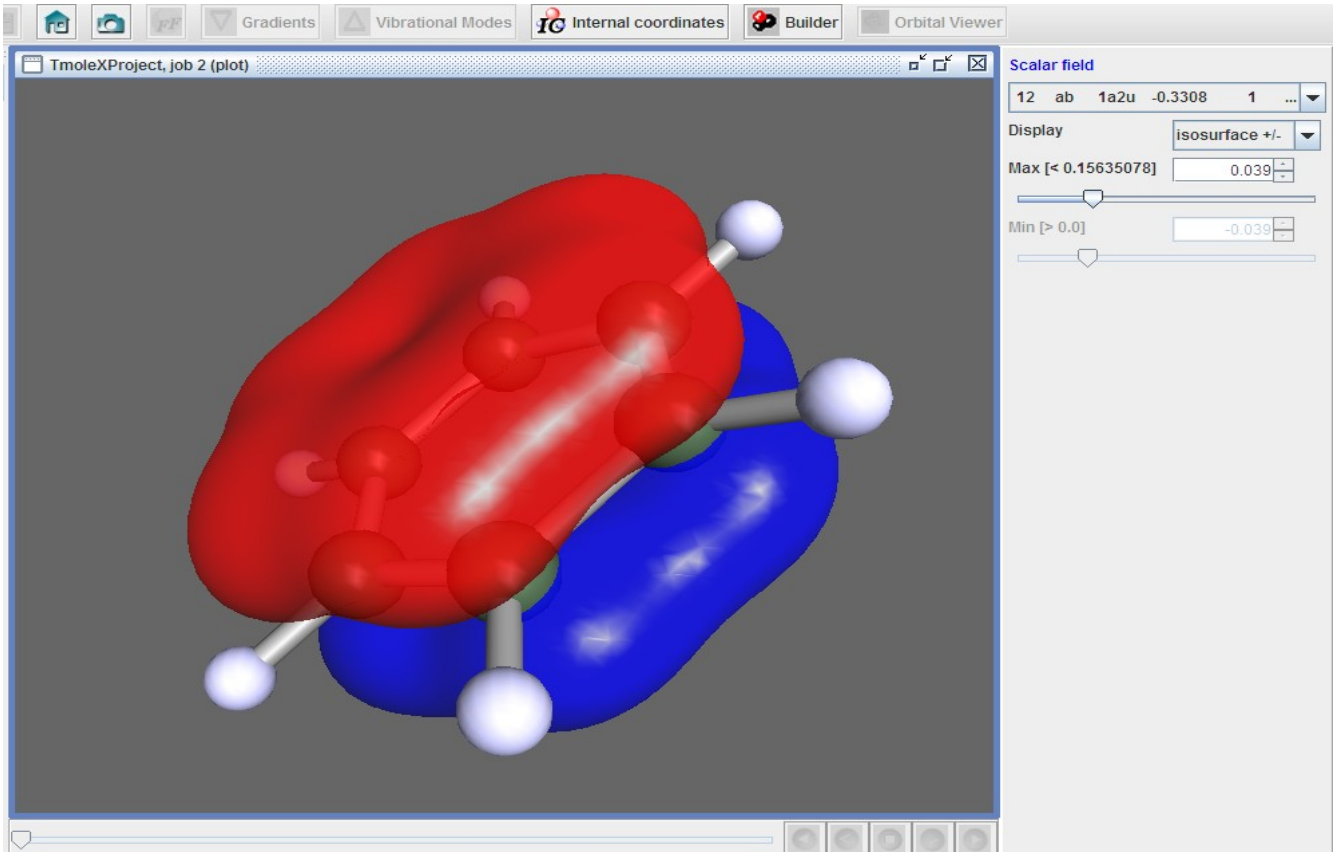
Click on Next to proceed. A progress bar is shown:



If you choose several options like orbitals, densities, electrostatic potential, etc., each property will have its own progress bar. All properties which require solving integrals like electrostatic properties, densities and their derivatives, etc. are quite expensive. Especially for larger molecules, generating 3D plot files can take (much) longer than the single-point calculation or a geometry optimization!

When the calculation is finished, the orbitals or property can be selected for visualization. Several properties can be displayed in the same window. Check the memory usage of TmoleX from time to time when using this option!


3D-Visualizer
Open the Viewer with the Following Property
Choose orbital
No. Spin Symmetry Energy[H] Degeneracy Occupancy
19 ab 19a 0.065 1 0
18 ab 18a 0.0233 1 0
17 ab 17a -0.1975 1 2
16 ab 16a -0.2208 1 2
Choose property to view
Open in Last Window
Open in New Window
Cancel
Back
Generate New Property



There are a lot of options and possibilities when visualizing 3D surfaces. The most important things are:

- while it can be annoying that the full 3D grid is being calculated, which can be very time consuming, TmoleX can now use this data to generate the 2D surface for a given iso-value on-the-fly.
  Use the slider or the field for the iso-value to change the threshold.
- The 'Display' options are:
  - isosurface – use one iso-value to plot the surface at this value
  - cloud – plot each point of the 3D grid which is within the Min and Max value. The colours of the points depend on the Min-Max range.
  - Isoplot – plot a plane (or an arbitrary surface which can be given as implicit equation like x^2+y^2+z^2-4. Avoid blanks and let the mouse pointer rest over the field to get some help) coloured with the value of the chosen property. Colour depends on the Min-Max range. If you see nothing, not enough, or not enough colours, change Min and/or Max value.
  - Isoplot again – click 'on isosurface' and a file chooser will open. Click on e.g. td.plt (total density) and set an iso-value below. This will result in a 2D surface which represents the iso-value of the density

and the colour on the surface is given by the value of the chosen property at that points. Typical example: open electrostatic potential, use the isoplot option, choose td.plt for the total density and set an iso-value. This will give a typical picture of a electrostatic potential on an density-isosurface.

- Isosurface +/- – plots two iso-densities: one at the positive value and one at the negative value. A typical molecular orbital picture.

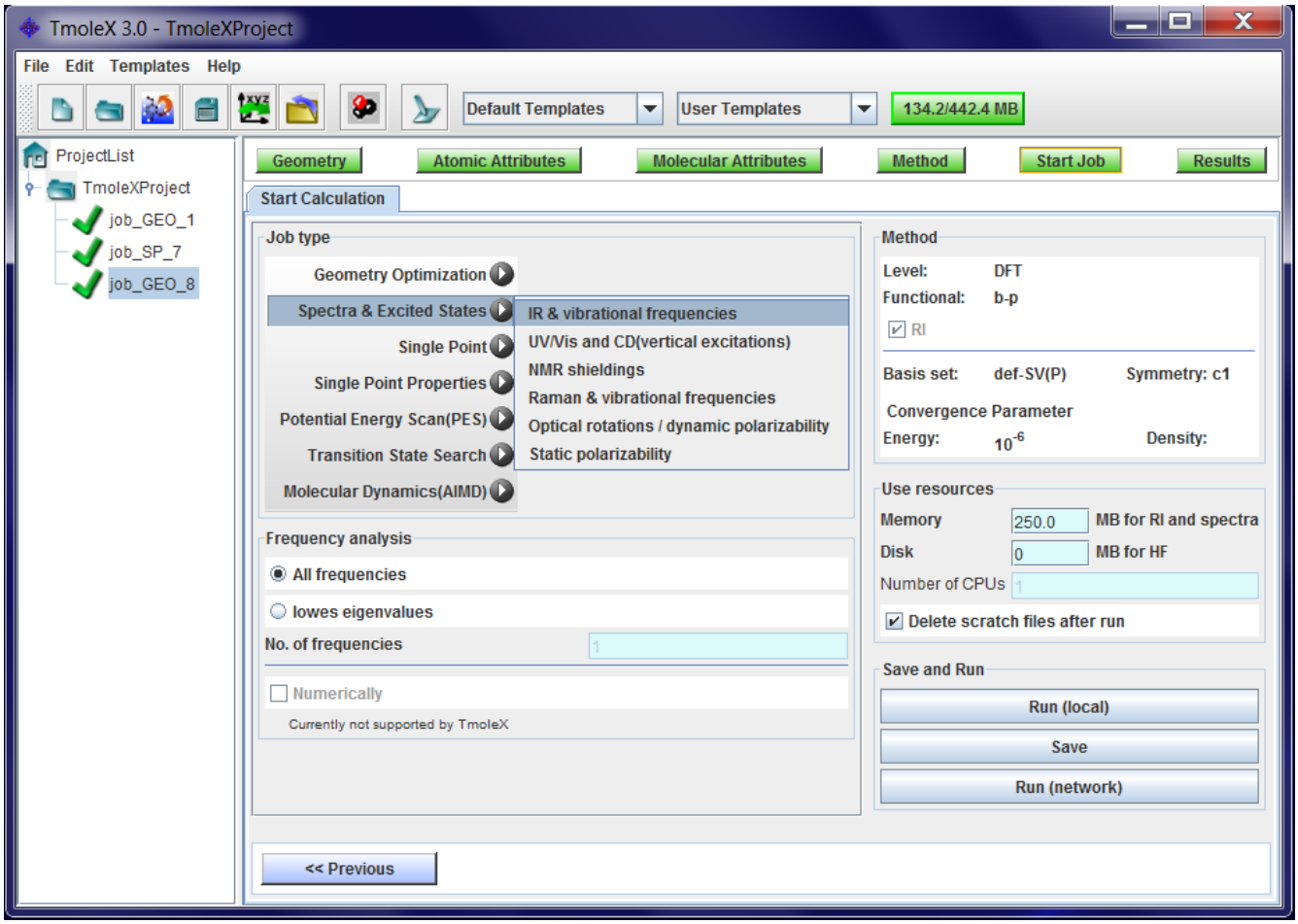
Vector plots

Vector fields can be visualized too, the best way to get an idea of the field depends on the property. Most options are similar to those described above.

4. Properties

4.1. Vibrational frequencies

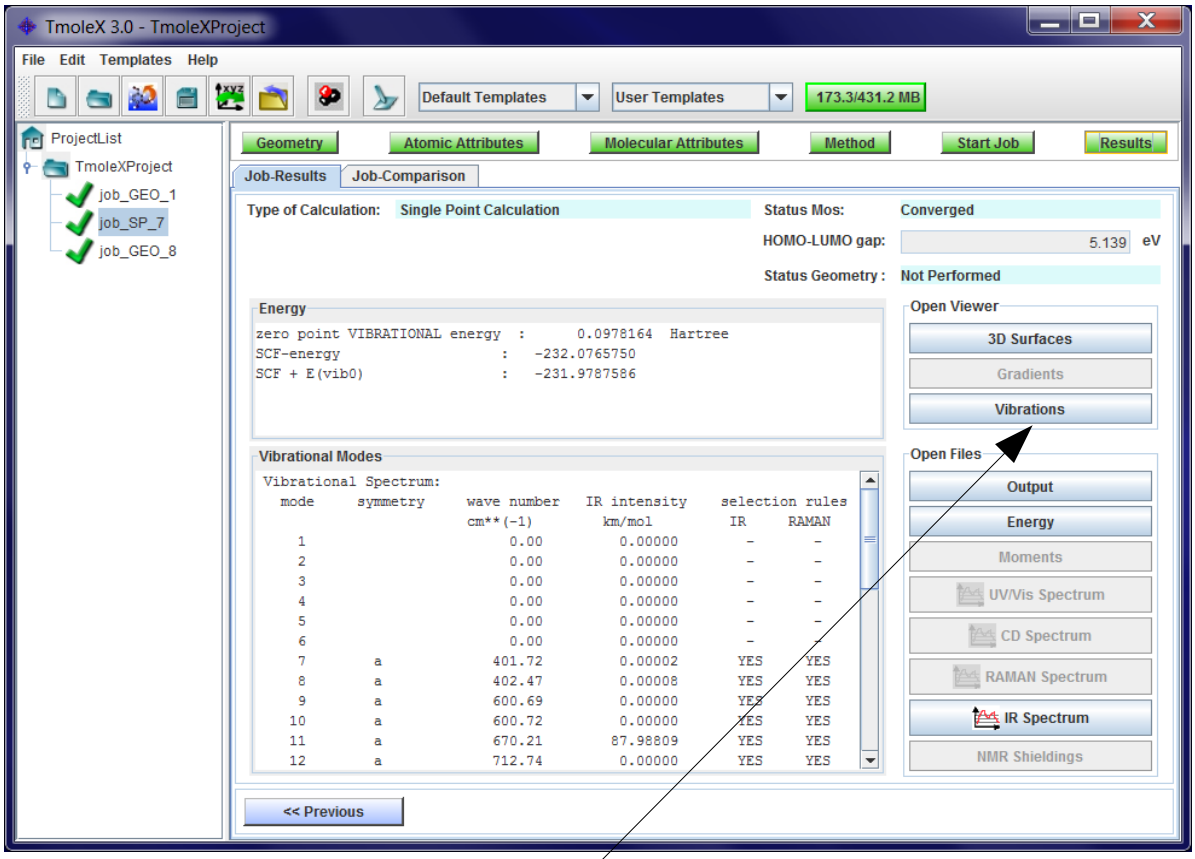
If you have an optimized geometry, you might want to follow it up by a frequency calculation, either in order to check, if you are in minimum, or because you are interested in the IR spectrum.



Choose 'IR & vibrational frequencies' in the 'Start Job' panel and click on Run.

4.Properties

The IR spectrum can be found in the 'Results' panel.

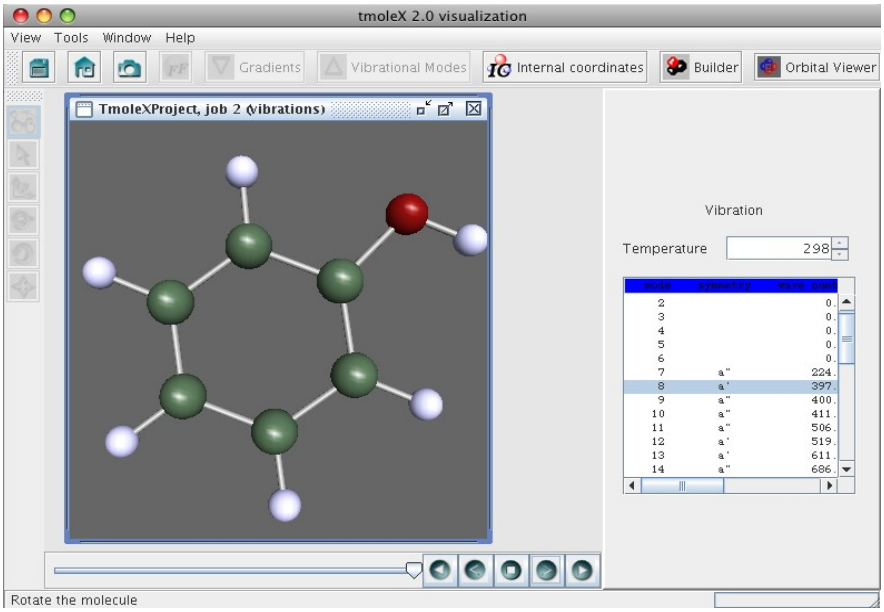


You can look at the mode in the 3D visualization.

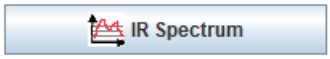
Select a specific mode and click 'play'.

Temperature sets the amplitude.

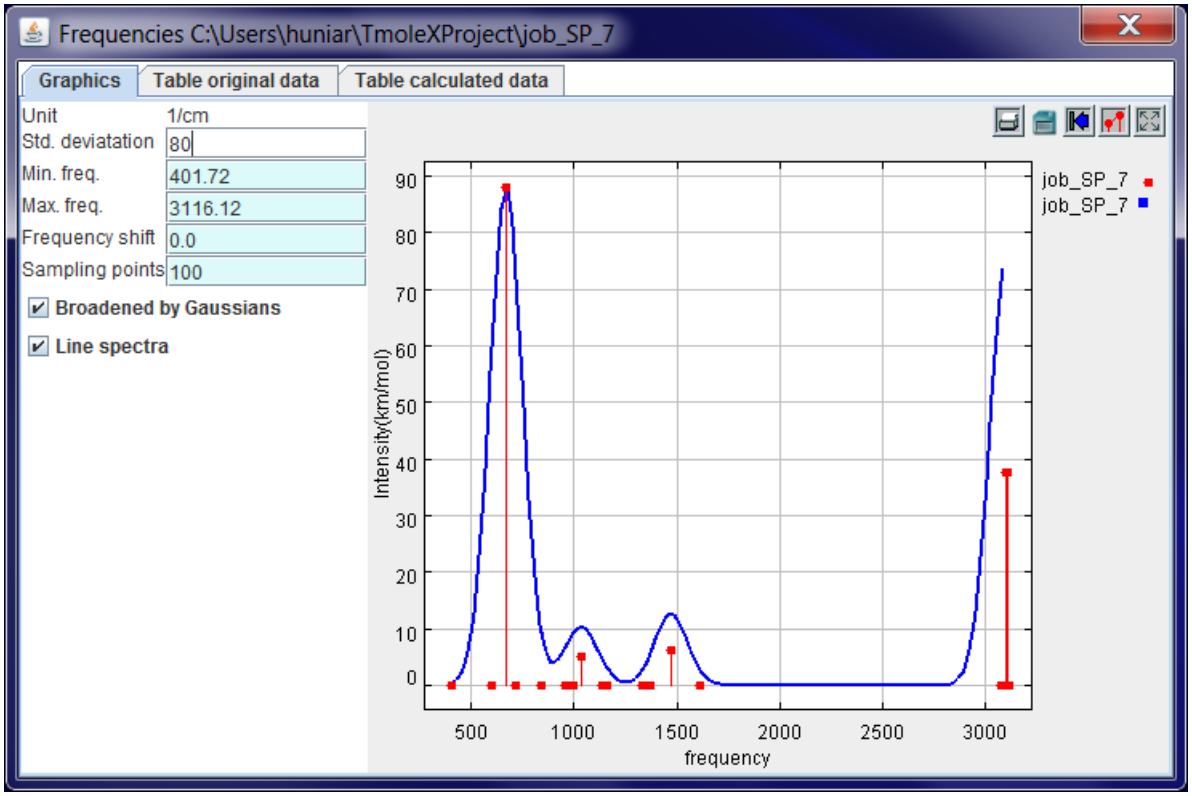
Use the play buttons and/or the slider to see the mode.



4.2. IR spectrum

Use the 

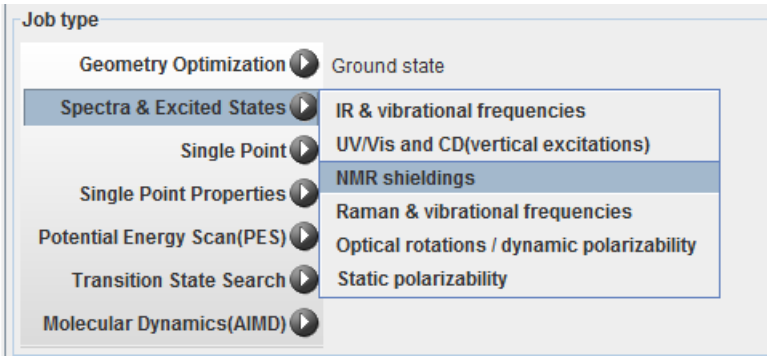
to open the IR spectrum:



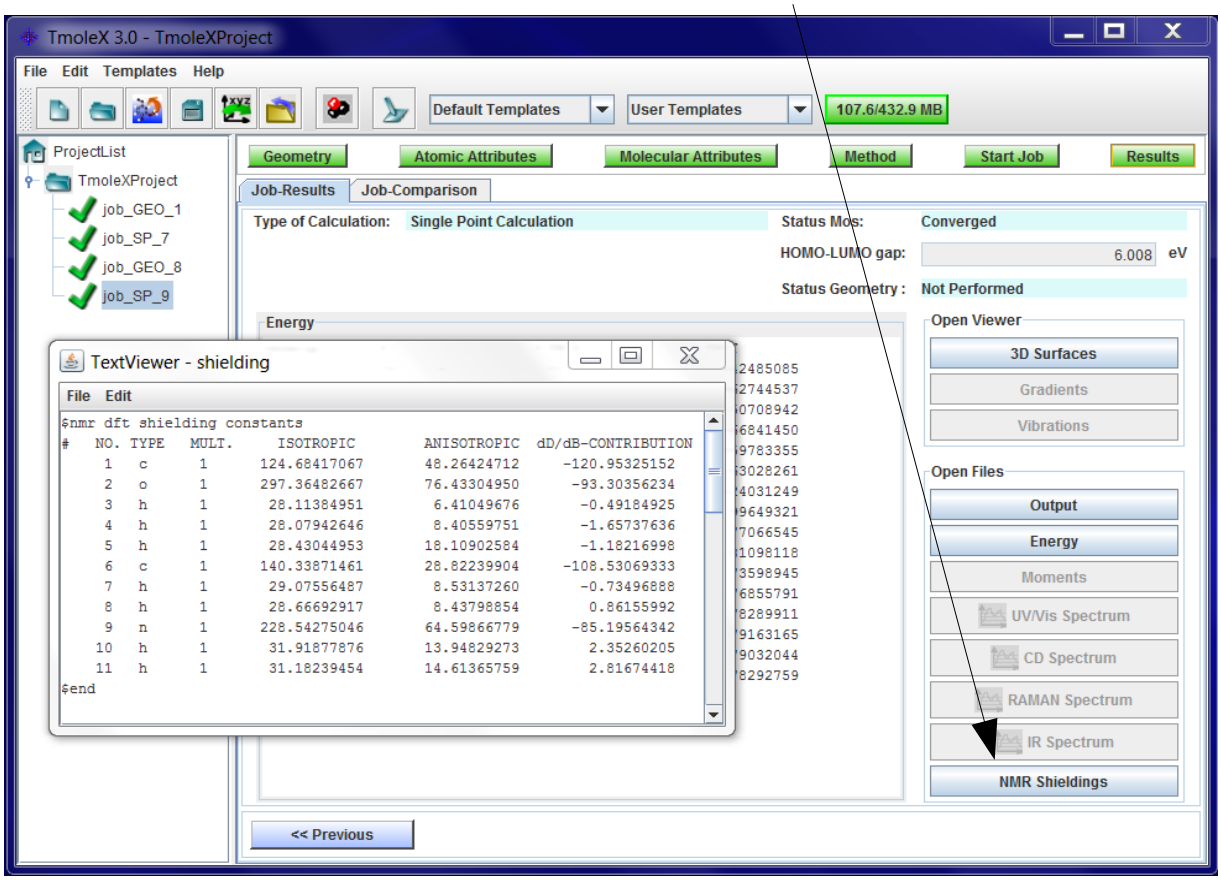
Standard deviation for the broadening Gaussians, a frequency shift, number of sampling points, etc. can be entered. The tables with the original data (line spectrum) and calculated data (points that define the broadened lines) can be used to copy and paste the data to a spread sheet or a statistics program.

4.3. Nuclear magnetic shielding

For the calculation of nuclear shieldings choose this job type and simply run it.



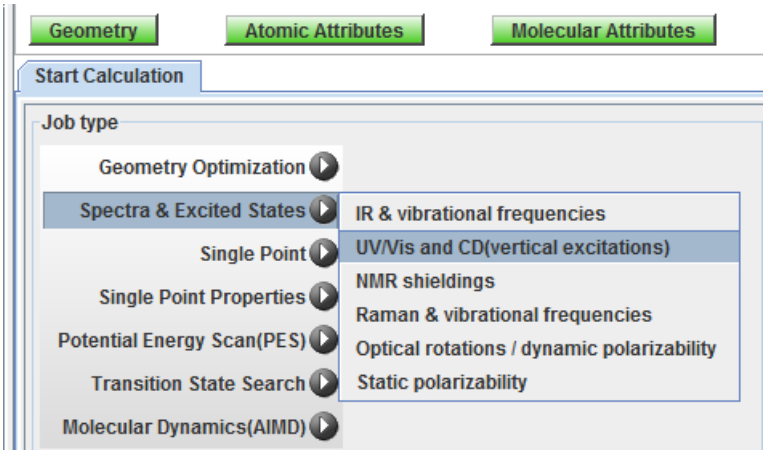
In the 'Results' panel you can open the shielding constants in a text viewer.



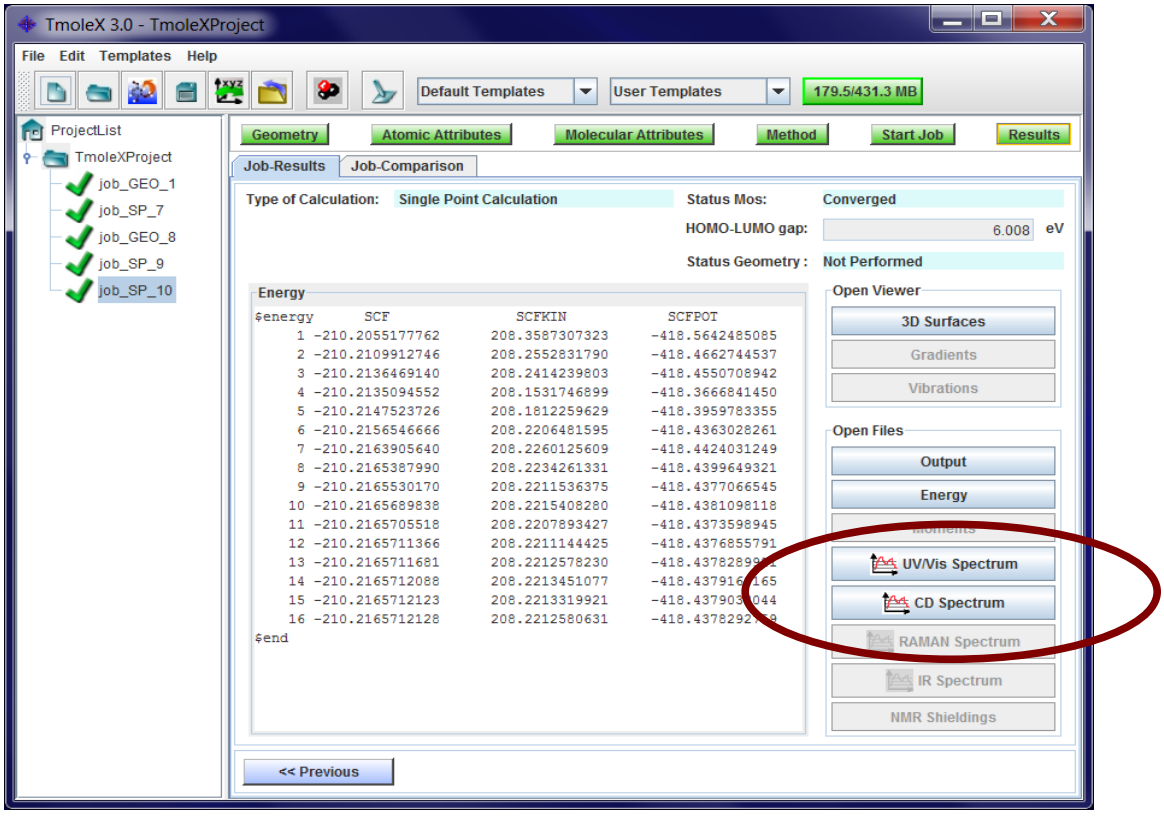
Copy and paste the values to a spread sheet for further usage. Note that to get the NMR shifts, you have to do a calculation also on the reference molecule (like TMS for carbon) with the same method and basis set.

4.4. UV/Vis and CD spectra (TD-DFT)

A TD-DFT calculation is set up like a normal DFT calculation. Then choose 'Excited States' in the job selection, select singlet or triplet, the number of excitations, and run it.



The spectra can be opened with the CD or UV/Vis Spectrum button.



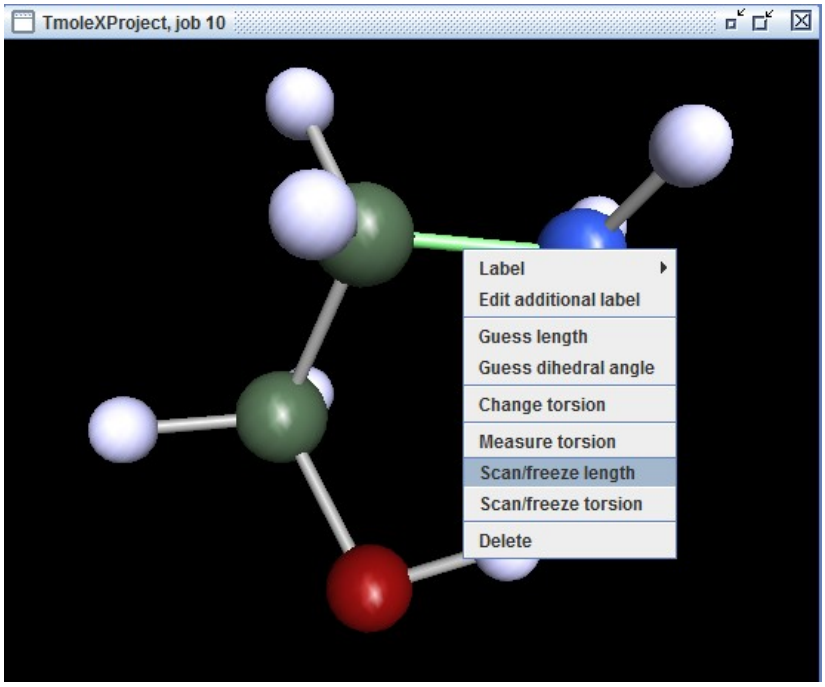
5. Constrained optimization and Scan jobs

5.1. Defining fixed internal coordinates

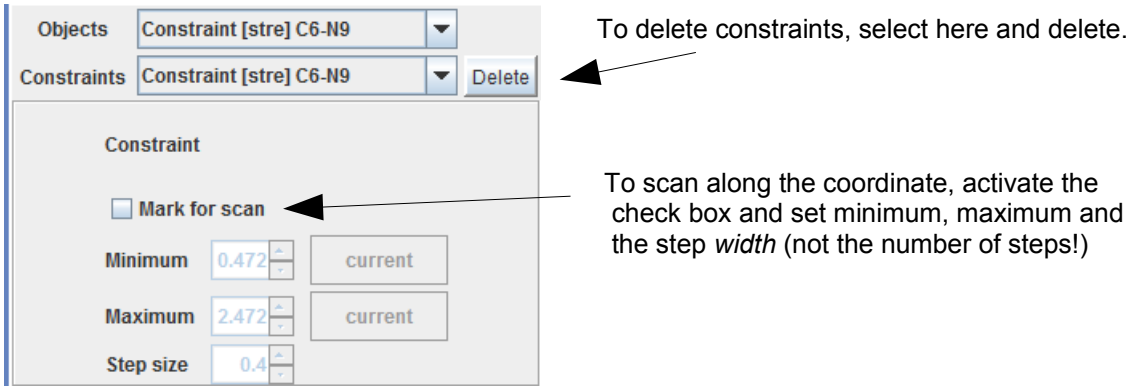
TmoleX 3 introduces a new way to define internal coordinates. Bonds, bond angles and torsions can be fixed within the builder.

To define a constraint, select one, two or three bonds:

- select one bond, click on the right mouse and choose Scan/freeze length:

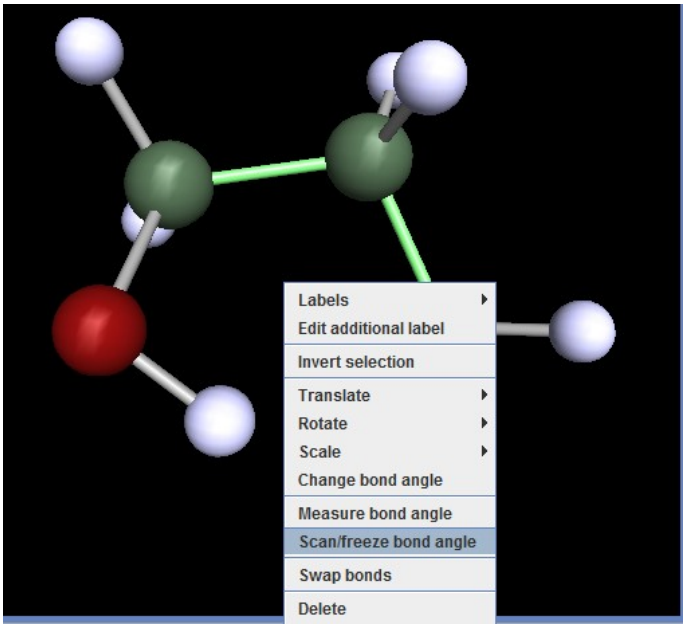


On the right the options for freezing a bond length are show:



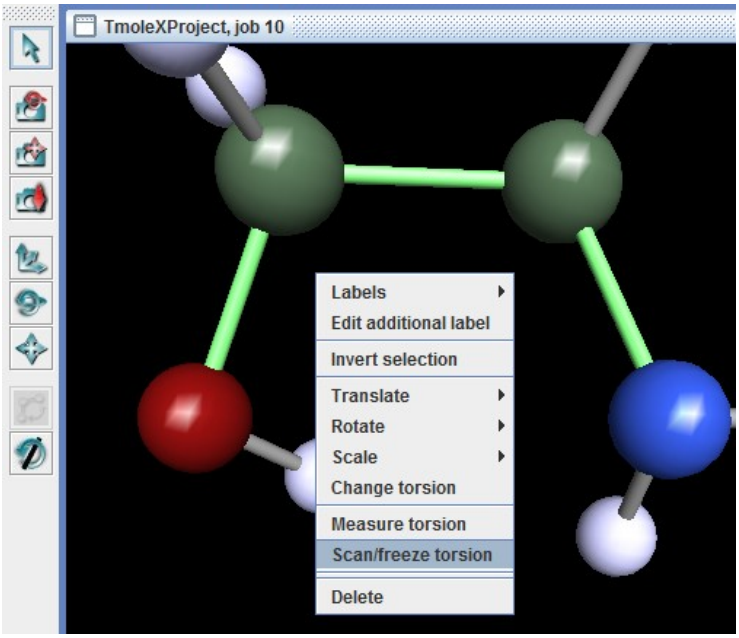
5.1.Defining fixed internal coordinates

- Select two adjacent bonds, click on the right mouse button and use the Scan/freeze bond angle option:



  Again, on the right side you will get the same options for scan jobs as shown above.

- Select *one or three* bonds to freeze a torsion. If you just select one, TmoleX will take just one of the possible torsional angles. If you use the 'Change torsion' or the corresponding button on the left side of the window, the value of the internal coordinate is shown and can be changed as usual with dragging the mouse while keeping the left mouse button pressed.



5.2. Use internal coordinates

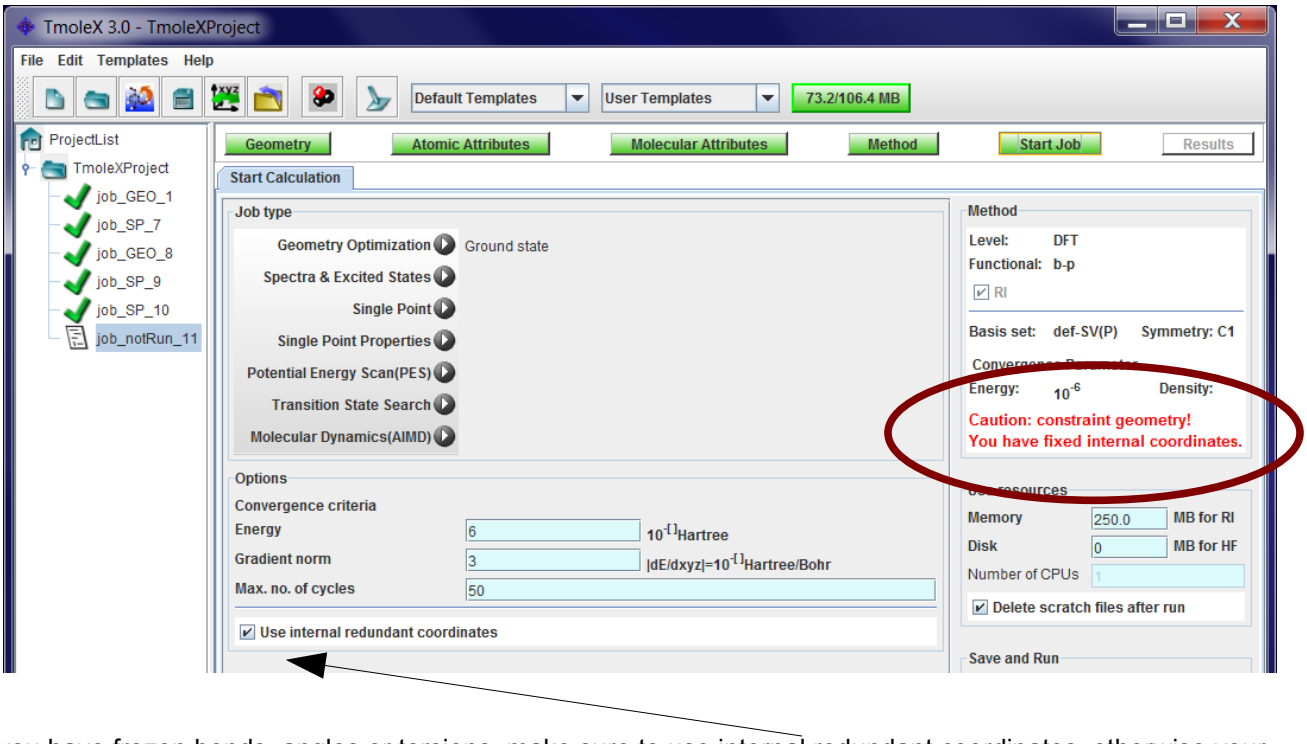
TmoleX will automatically generate a list of internal redundant coordinates if you accept that when being asked for. If you use constraints or scan jobs, internal redundant coordinate usage must be activated when starting a geometry optimization!

Be careful with linear combinations (several lines of definitions for one internal coordinate) – while they can be fixed, this is usually not what one really wants!

There is a possibility to visualize the set of internal redundant from within the Geometry panel.

5.3. Start constrained optimization

A constrained search is automatically done if a usual geometry optimization job is started while having internal (or Cartesian) coordinates fixed. TmoleX will show a message in the panel where such jobs are started:



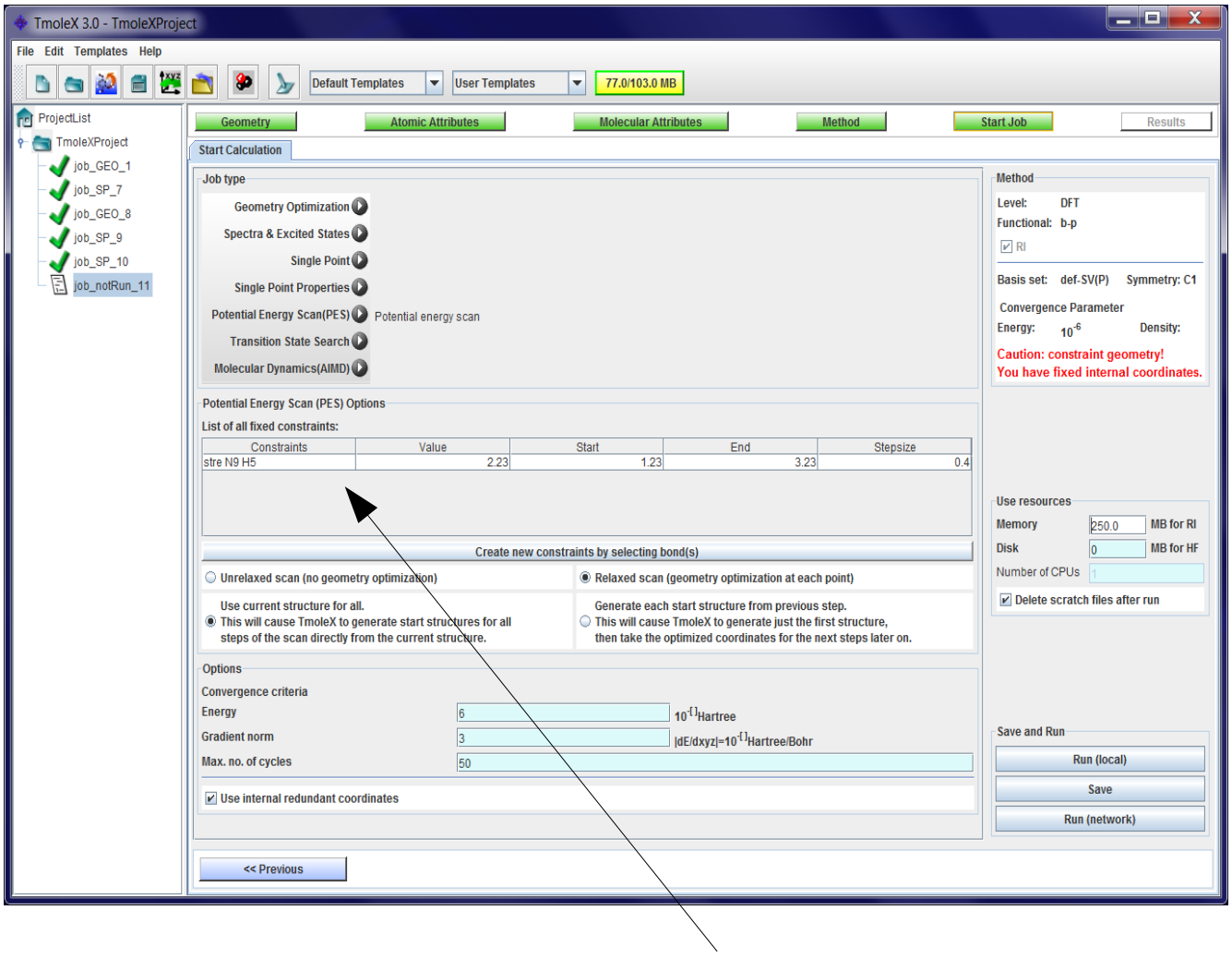
If you have frozen bonds, angles or torsions, make sure to use internal redundant coordinates, otherwise your settings will be ignored!

Constrains are always applied in this section, no matter if ground or excited states calculations are done, minimum search (geometry optimization), potential energy scans, or transition state searches are started.

5.4. Scan along an internal coordinate

The potential energy scan (PES) method can be applied if internal coordinates are defined, and at least one of them is defined as fixed. Scan will run a couple of geometry optimizations for a range of values of an internal coordinate.

Note that **all** fixed internal coordinates will be kept fixed, not just the one that you have defined to be scanned along! For a one-dimensional scan job, only one internal coordinate should be defined as fixed.



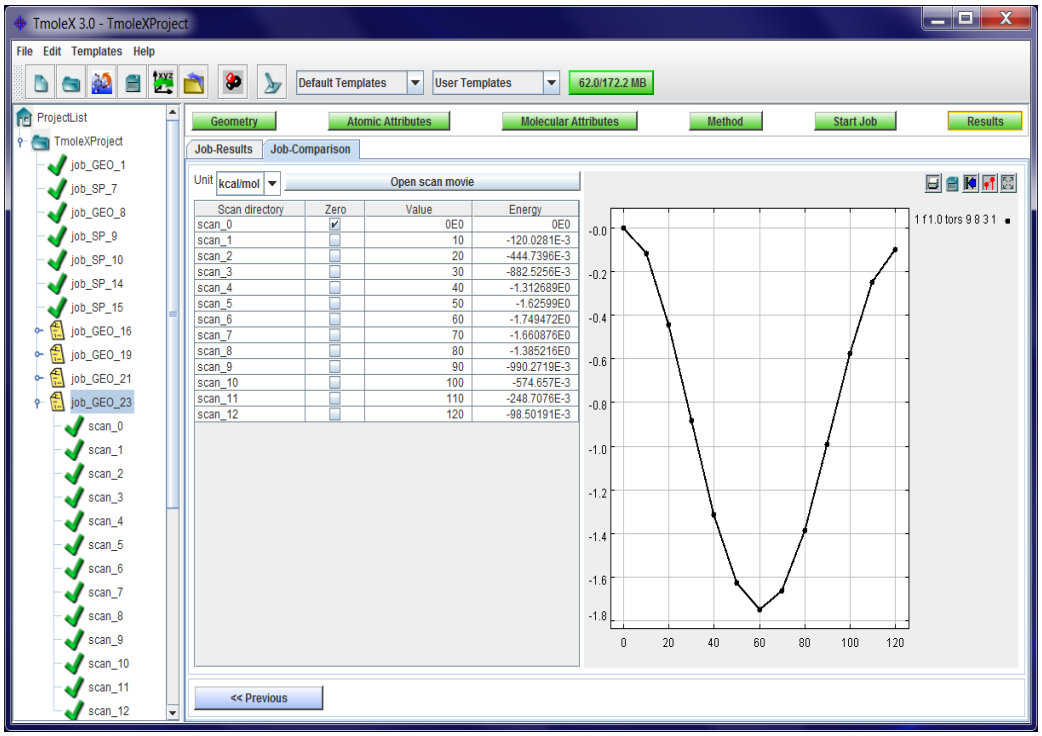
The list of fixed internal coordinates is shown in the PES scan Options section. To define a new fixed internal coordinates, use the Create new constraints by selecting bond(s) button. This is not needed if you did that in the builder already.

The different options how the start geometries are generated are described in the panel itself.

Unrelaxed scans and relaxed scans are possible (single-point or geometry optimization calculations will be done).

We recommend to use the 'Use current structure for all' option, because if one of the steps fail, the remaining jobs will have problems too otherwise.

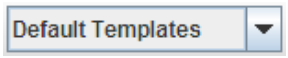
The job can then be started as usual, also as a remote calculation. A typical result is shown here:



The final optimized structures are stored for each of the scan points in a multi-coord file – similar to the gradient view. This can be viewed like a movie with the button Open scan movie.

6. Templates

TmoleX gives you the possibility to save the most important settings of your jobs like basis set, method or job type to a template. This helps to reduce the time needed for an input preparation if the same kind of job has to be performed for a set of molecules.

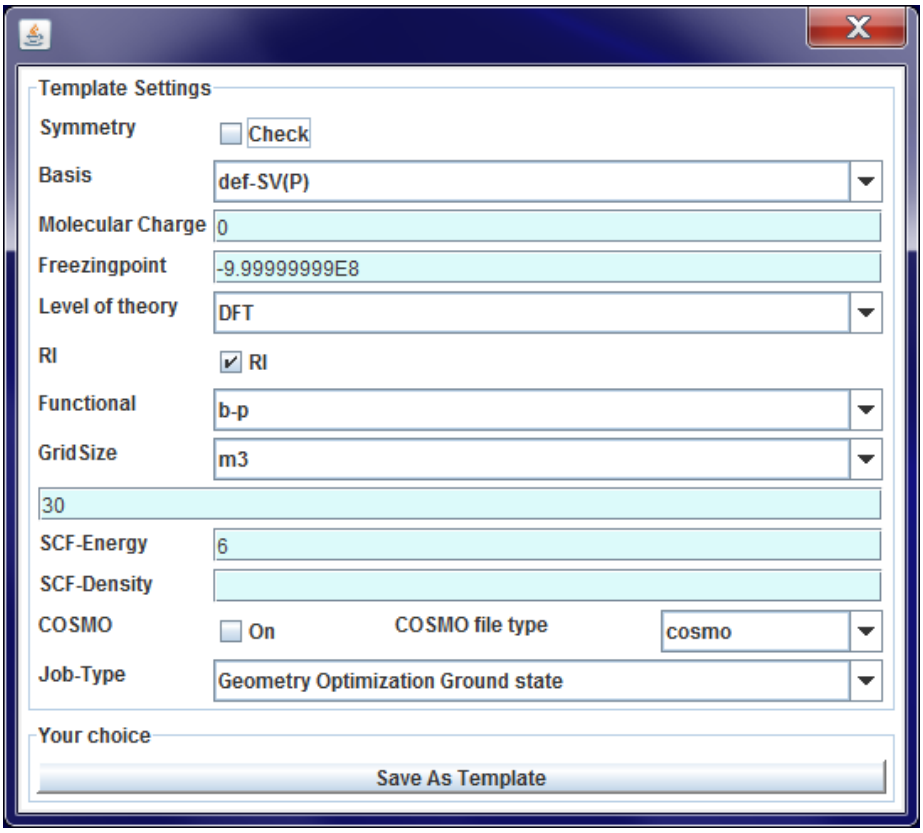
To use a template, just choose a saved template from either 

or

.

TmoleX will alter the settings accordingly, generate start orbitals, and brings you directly to the start-job panel.

To save a template, choose 'Save template' from the Template menu of TmoleX.



The settings are quite self-explaining, but at this point, *TmoleX does not check for consistency* of different settings. So please do first a usual job, run it, and check if the combinations are possible (e.g. 2nd derivatives for post-Hartree-Fock methods are not supported by TmoleX, excited states with TPSS are generally not possible, COSMO calculations and frequency analysis is not supported either, etc.).

The template will have to be named when saving and can be found in the

pull-down menu afterwards.

7. Remote jobs

TmoleX as well as the client version of TmoleX which is freely available from COSMOlogic web site is able to start jobs on remote Linux/Unix machines using a secure shell.

7.1. Security information

To determine if you do want to use this feature and worry about security, here is a short outline of the procedure used by TmoleX to access to remote systems.

- ssh and scp are used to start jobs and to copy the files from one system to another.

  We use a locally modified version of PuTTY (http://www.chiark.greenend.org.uk/~sgtatham/putty/)

  PuTTY is copyright 1997-2009 Simon Tatham.

  Portions copyright Robert de Bath, Joris van Rantwijk, Delian Delchev, Andreas Schultz, Jeroen Massar, Wez Furlong, Nicolas Barry, Justin Bradford, Ben Harris, Malcolm Smith, Ahmad Khalifa, Markus Kuhn, Colin Watson, and CORE SDI S.A.

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- PuTTY uses its own repository for public ssh keys, so ssh connections that do not require a password on your local machine at the command line might not work if OpenSSH or any other ssh program is used. Run ssh from the TmoleX directory to check that manually.

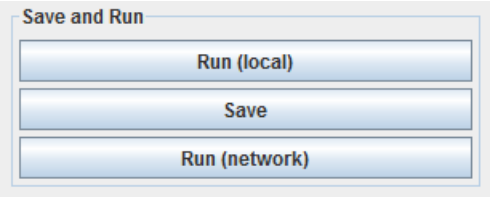
- jobs can be killed while they run on a remote system. For that purpose, a kill-job script is being stored in the directory where the job is running. This script does kill all processes that are running in the directory the script itself is located – but this will only work on systems where a /proc directory is present (usually all Linux systems and most Unix systems either).

- Passwords entered in the password field **will not be saved** to disk. Hence, they have to be entered each time TmoleX has been started, but kept in memory as long as TmoleX runs.

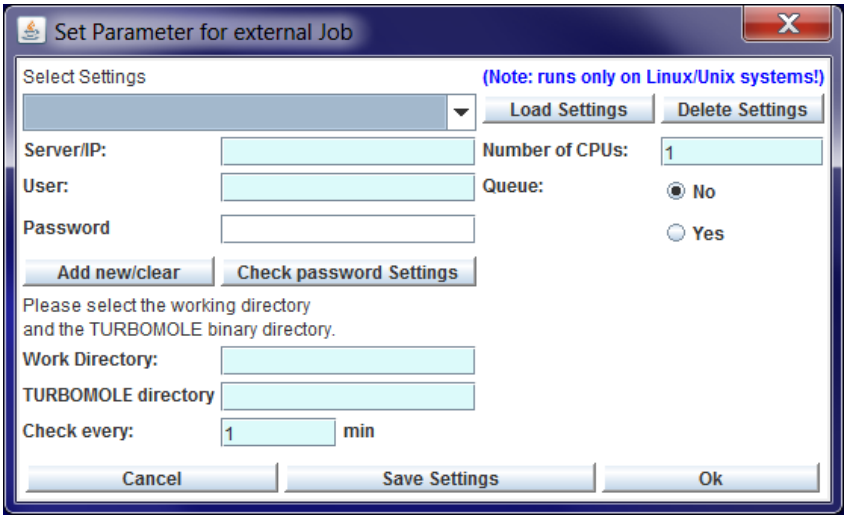
7.2. Add new remote machine

When starting a remote job for the first time, or when you want to add several external machines, several things have to be set, TmoleX needs to know in order to be able to run TURBOMOLE there.

To start a job on a remote machine, or to set or change settings, click on Run (network) in the 'Start Job' panel.



TmoleX will first save the input file to a local disk under the usual naming scheme, and then open a new window that looks like this one:



General informations about a remote system are:

1. The name or the IP address of a remote machine (Server/IP field)
2. User name on that machine
3. Password to log in

Those three field have to be filled in first. To check if the settings are correct, and if a connection can be established, click on Check password Settings. TmoleX will try to log in and determine the home directory of the user which has been given in the User field.

If the connection has been successful, the home directory will be added to the 'Work Directory' field.

4. Work directory tells TmoleX in which path on the remote machine the job shall run – a local fast disk should be chosen here.

5. TURBOMOLE directory has to be set to the TURBOMOLE installation directory on the target system.

   The default behaviour of ssh when starting remote jobs without an explicit shell or terminal is such that not all settings on the remote system are sourced. So it is very likely that your TURBOMOLE settings (like $TURBODIR, $PATH, etc) are not available in such a case.

   It is therefore unavoidable to set the PATH to the TURBOMOLE directory on the remote system by hand.

6. The number of CPUs can be left unchanged.

   Note that this field is not to tell TmoleX how many CPUs or cores are available in general, but how many CPUs shall be used for the calculation of each job!

7. Note that all jobs are started on the remote system with nohup. TmoleX does not get a notice when the job has finished, so it has to check actively if the job is still running or not. The frequency for those checks can be given in minutes.

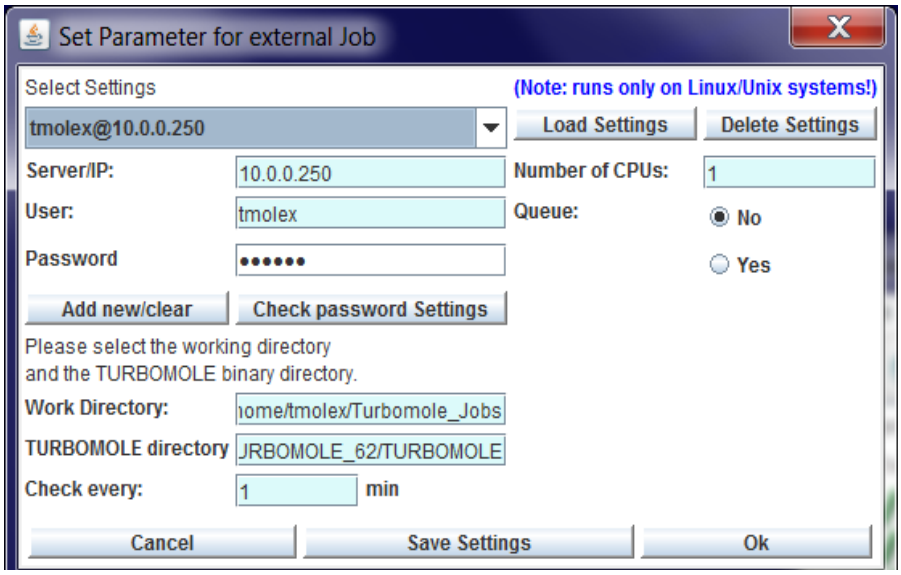
8. The queueing system option can be used to submit remote jobs to a queue which is accessible on the remote machine.

After settings 1-5 are complete, click on

, and the machine with user name and paths will be suggested as name which will be added to the pull down list of machines for future usage.

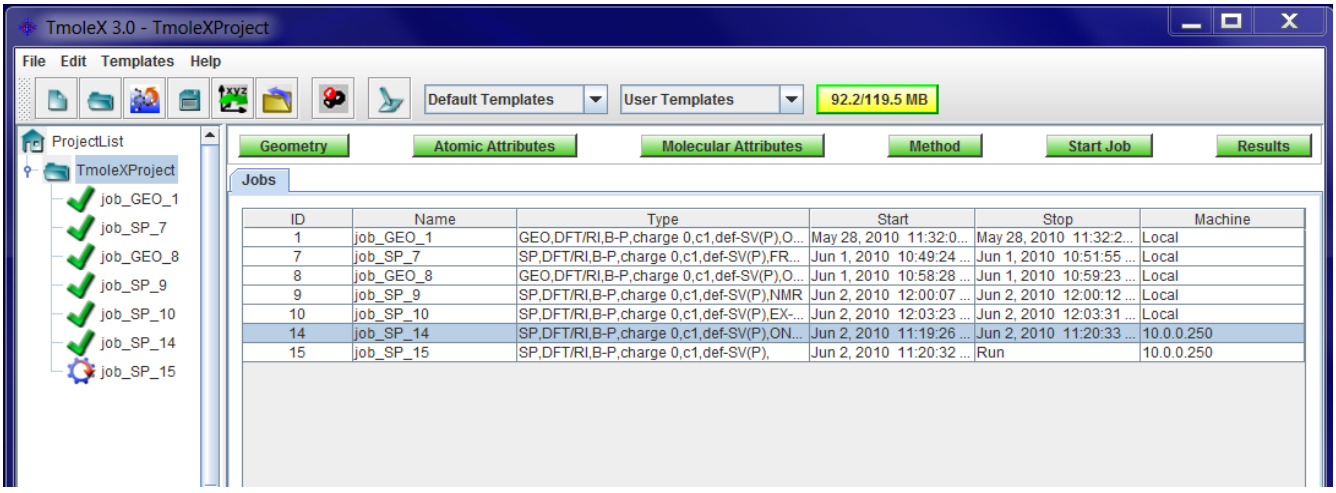
7.3. Start a remote job

Starting jobs can be done by choosing a machine in the list of saved systems:



A simple click on Ok will start the job on the chosen system.

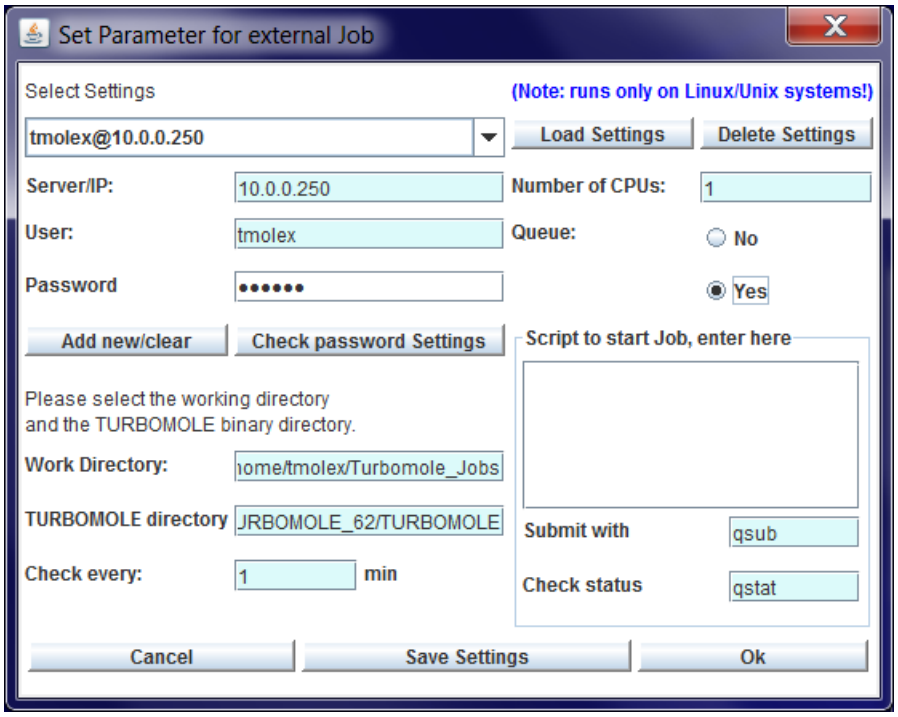
The job list shows on which machine a calculation has been started or is still running. The right mouse button menu in this list allows to kill a job also on a remote machine.


TmoleX 3.0 - TmoleXProject
File Edit Templates Help
Default Templates
User Templates
92.2/119.5 MB
ProjectList
TmoleXProject
job_GEO_1
job_SP_7
job_GEO_8
job_SP_9
job_SP_10
job_SP_14
job_SP_15
Geometry
Atomic Attributes
Molecular Attributes
Method
Start Job
Results
Jobs
ID Name Type Start Stop Machine
1 job_GEO_1 GEO,DFT/RI,B-P,charge 0,c1,def-SV(P),O... May 28, 2010 11:32:0... May 28, 2010 11:32:2... Local
7 job_SP_7 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),FR... Jun 1, 2010 10:49:24 ... Jun 1, 2010 10:51:55 ... Local
8 job_GEO_8 GEO,DFT/RI,B-P,charge 0,c1,def-SV(P),O... Jun 1, 2010 10:58:28 ... Jun 1, 2010 10:59:23 ... Local
9 job_SP_9 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),NMR Jun 2, 2010 12:00:07 ... Jun 2, 2010 12:00:12 ... Local
10 job_SP_10 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),EX-... Jun 2, 2010 12:03:23 ... Jun 2, 2010 12:03:31 ... Local
14 job_SP_14 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),ON... Jun 2, 2010 11:19:26 ... Jun 2, 2010 11:20:33 ... 10.0.0.250
15 job_SP_15 SP,DFT/RI,B-P,charge 0,c1,def-SV(P), Jun 2, 2010 11:20:32 ... Run 10.0.0.250

Note that the Stop time is not the end of the job itself, but the time when TmoleX noticed that the job has finished!

7.4. Using a queuing-system

Currently PBS and LSF are successfully tested. Activate the queue option in the remote job start panel:



To be able to support as many queuing systems as possible, the number of options is kept very small.

1. Submit with – this is the command that is used on the given remote system to submit a job to the queue. Here you can give just the name but also options.

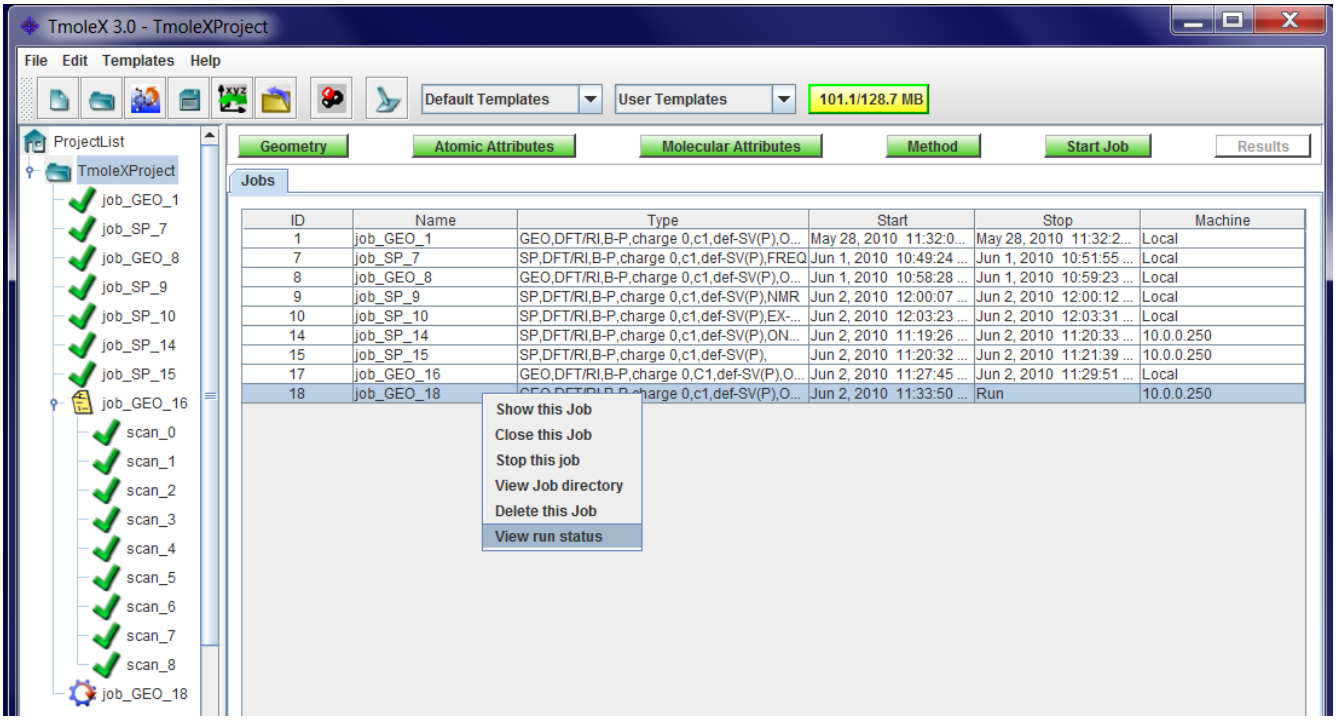
   For PBS,

   ```
   qsub
   ```

   is the default. For LSF it should be:

   ```
   bsub <
   ```

2. Check status – this is the command that is called on the remote system if the 'View run status' option from the right-mouse menu of the Job administration is chosen:


TmoleX 3.0 - TmoleXProject
File Edit Templates Help
Default Templates
User Templates
101.1/128.7 MB
ProjectList
TmoleXProject
job_GEO_1
job_SP_7
job_GEO_8
job_SP_9
job_SP_10
job_SP_14
job_SP_15
job_GEO_16
scan_0
scan_1
scan_2
scan_3
scan_4
scan_5
scan_6
scan_7
scan_8
job_GEO_18
Geometry
Atomic Attributes
Molecular Attributes
Method
Start Job
Results
Jobs
ID Name Type Start Stop Machine
1 job_GEO_1 GEO,DFT/RI,B-P,charge 0,c1,def-SV(P),O... May 28, 2010 11:32:0... May 28, 2010 11:32:2... Local
7 job_SP_7 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),FREQ Jun 1, 2010 10:49:24 ... Jun 1, 2010 10:51:55 ... Local
8 job_GEO_8 GEO,DFT/RI,B-P,charge 0,c1,def-SV(P),O... Jun 1, 2010 10:58:28 ... Jun 1, 2010 10:59:23 ... Local
9 job_SP_9 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),NMR Jun 2, 2010 12:00:07 ... Jun 2, 2010 12:00:12 ... Local
10 job_SP_10 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),EX-... Jun 2, 2010 12:03:23 ... Jun 2, 2010 12:03:31 ... Local
14 job_SP_14 SP,DFT/RI,B-P,charge 0,c1,def-SV(P),ON... Jun 2, 2010 11:19:26 ... Jun 2, 2010 11:20:33 ... 10.0.0.250
15 job_SP_15 SP,DFT/RI,B-P,charge 0,c1,def-SV(P), Jun 2, 2010 11:20:32 ... Jun 2, 2010 11:21:39 ... 10.0.0.250
17 job_GEO_16 GEO,DFT/RI,B-P,charge 0,C1,def-SV(P),O... Jun 2, 2010 11:27:45 ... Jun 2, 2010 11:29:51 ... Local
18 job_GEO_18 Jun 2, 2010 11:33:50 ... Run 10.0.0.250
Show this Job
Close this Job
Stop this job
View Job directory
Delete this Job
View run status

The output of the status command is shown directly underneath the job list.

3. Script to start Job, enter here

   This is the field where a usual script that is used to submit jobs to a queue can be entered. Example:

```
#Name of your run :
#PBS -N TmoleX-job
#Number of nodes to run on:
#PBS -l nodes=1
#
# Export environment:
#PBS -V

cd $PBS_O_WORKDIR
```

   This is a PBS example for a serial run.

   There are several things one has to take care of. TmoleX will use the given entry and include it in its own settings:

   1. do not give a `#!/bin/...` line here, TmoleX adds its own commands in sh format, so TmoleX will add a first line containing `#!/bin/sh` to the final script.

   2. Make sure to change the directory to where the input files are copied:

PBS:
```
cd $PBS_O_WORKDIR
```

LSF:

```
cd $LS_SUBCWD
```

must be somewhere in your own script.

3. Ask your queuing system for the right number of CPUs – this has to match the 'Number of CPUs' field of the TmoleX setting. Depending on the queuing-system, it will not allow a different number than what the script will start.

   $PARNODES is set by TmoleX, so if you set it in this field, it will be overwritten.

4. $TURBODIR is being set by TmoleX, so you do not have to enter it again here.

5. The commands to start the TURBOMOLE jobs are of course added by TmoleX automatically.